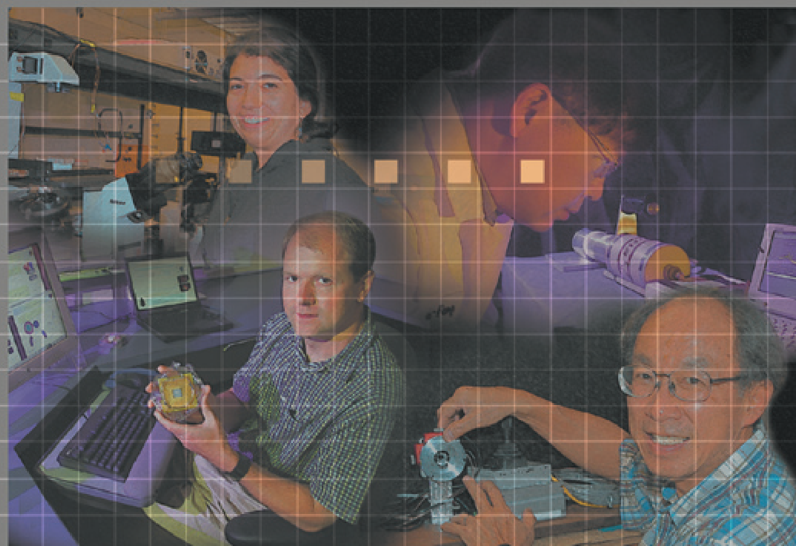
LAWRENCE LIVERMORE NATIONAL LABORATORY



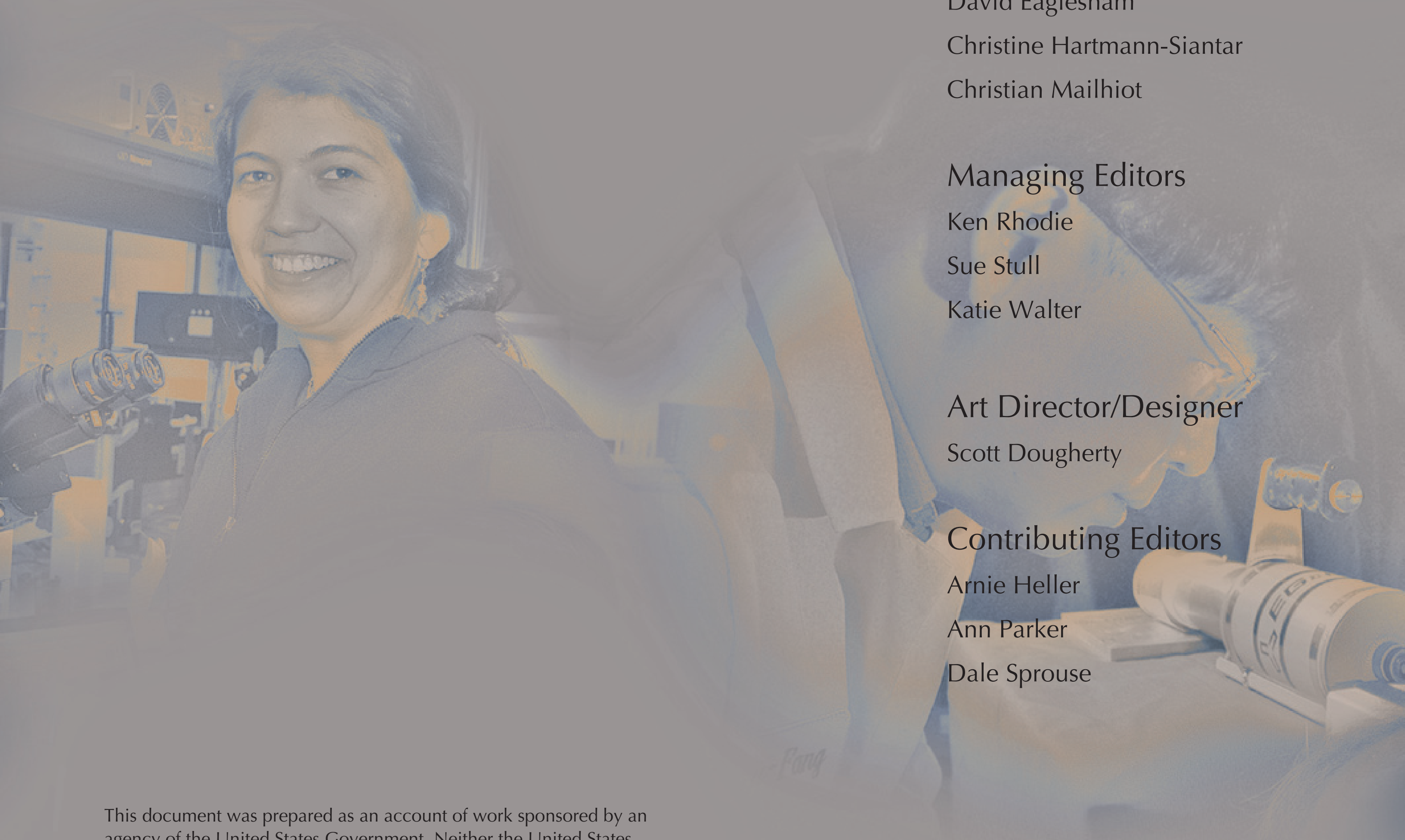
Chemistry and Materials Science
STRATEGIC PLAN

chemistry & materials science CMS

UCRL-TR-203305

Credits

A Web version of this strategic plan is available from the CMS Web site. The Plan site also includes information not presented in this document that is relevant to CMS strategic planning. The Plan Web site will be updated periodically to keep CMS employees apprised of important strategic planning issues and proposed future plans for the directorate.



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April 2004

In partnership with the rest of the Laboratory

The Full CMS Team is Needed to Successfully Execute the New Strategic Plan

The CMS Directorate Mission . . .

. . . is to enable Lawrence Livermore National Laboratory to accomplish its primary missions through excellence in the chemical and materials sciences.

The CMS Directorate Vision . . .

. . . is to be known as the premier provider of scientific leadership that meets and anticipates the needs of Laboratory programs, is recognized as a national leader in the chemical and materials sciences, and has an exceptional, safe, and secure work environment that attracts and retains a vital and diverse workforce.

The Laboratory's

mission is as clear today as it was in 1952 when the Laboratory was founded—to ensure our country's national security and the safety and reliability of its nuclear deterrent. As a laboratory pursuing applied science in the national interest, we strive to accomplish our mission through excellence in science and technology. We do this while developing and implementing sound and robust business practices in an environment that emphasizes security and ensures our safety and the safety of the community around us.

Our mission as a directorate derives directly from the Laboratory's charter. When I accepted the assignment of Associate Director for Chemistry and Materials Science (CMS), I talked to you about the need for strategic balance and excellence in all our endeavors. We also discussed how to take the directorate to the next level. The long-range CMS strategic plan presented here was developed with this purpose in mind. It also aligns with the Lab's institutional long-range science and technology plan and its 10-year facilities and infrastructure site plan.

The plan is aimed at ensuring that we fulfill our directorate's two governing principles: *(1) delivering on our commitments to Laboratory programs and sponsors, and (2) anticipating change and capitalizing on opportunities through innovation in science and technology.* This will require us to attain a new level of creativity, agility, and flexibility as we move forward. Moreover, a new level of engagement in partnerships with other directorates across the Laboratory as well as with universities and other national labs will also be required.

The group of managers and staff that I chartered to build a strategic plan identified four organizing themes that define our directorate's work and unite our staff with a set of common goals. The plan presented here explains how we will proceed in each of these four theme areas:

- **Materials properties and performance under extreme conditions**: Fundamental investigations of the properties and performance of states of matter under extreme dynamic, environmental, and nanoscale conditions, with an emphasis on materials of interest to Laboratory programs and mission needs.
- **Chemistry under extreme conditions and chemical engineering to support national security programs**: Insights into the chemical reactions of energetic materials in the nuclear stockpile through models of molecular response to extreme conditions of temperature and pressure, advancing a new technique for processing energetic materials by using sol-gel chemistry, providing materials for NIF optics, and furthering developments to enhance other high-power lasers.
- **Science supporting national objectives at the intersection of chemistry, materials science, and biology**: Multidisciplinary research for developing new technologies to combat chemical and biological terrorism, to monitor changes in the nation's nuclear stockpile, and to enable the development and application of new physical-science-based methodologies and tools for fundamental biology studies and human health applications.
- **Applied nuclear science for human health and national security**: Nuclear science research that is used to develop new methods and technologies for detecting and attributing nuclear materials, assisting Laboratory programs that require nuclear and radiochemical expertise in carrying out their missions, discovering new elements in the periodic table, and finding ways of detecting and understanding cellular response to radiation.

Interlaced throughout the discussion of the theme areas are goals and needs for plan implementation. Also, sidebars appearing in some of the theme-related sections and a closing section present examples of ways that this strategic plan is being implemented.

The needs and priorities of our directorate will inevitably change over time. Planning is an ongoing, ever-evolving endeavor. Therefore, my intention is to have the directorate continually engaged in strategic planning and to update our plans and strategies as new external forces push us into new and sometimes unexpected directions.

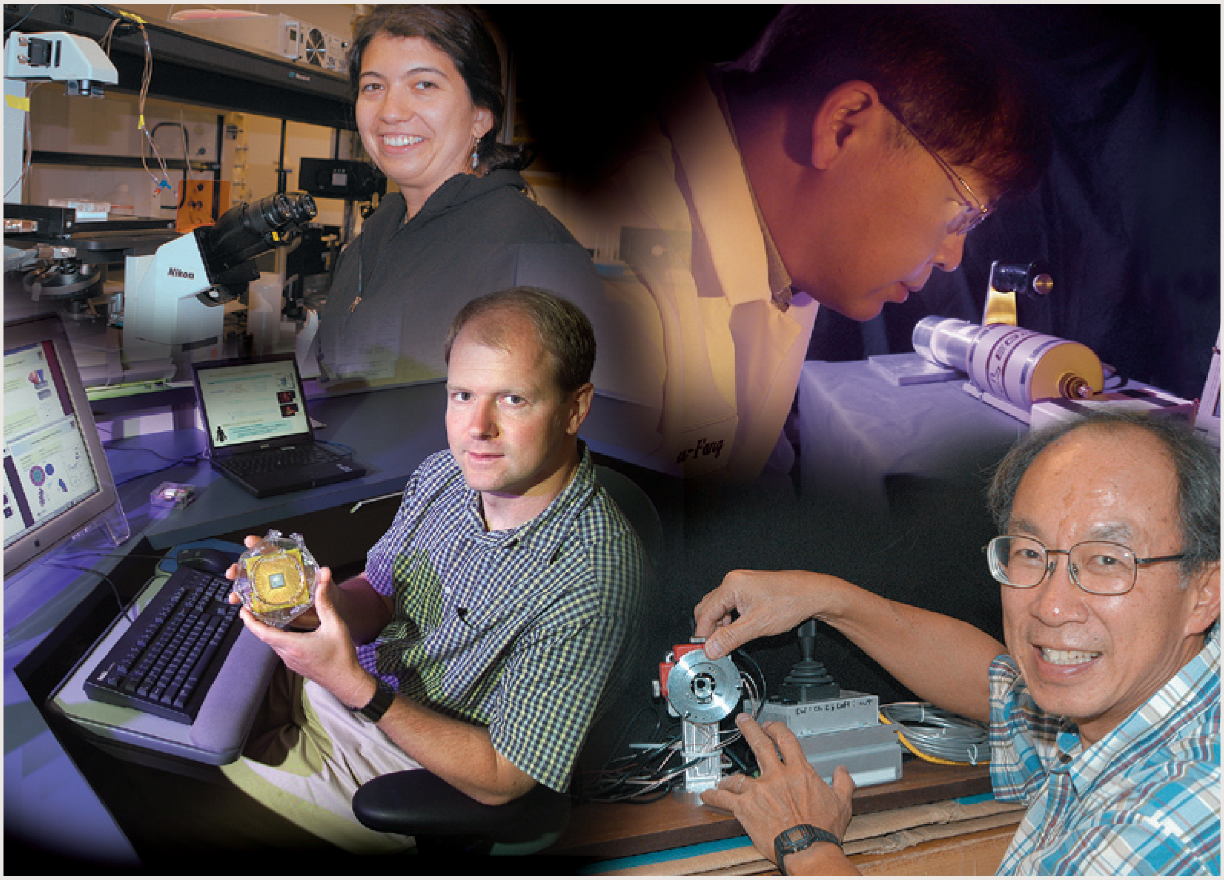
The CMS strategic plan focuses our efforts to support the Laboratory's national security and other emerging missions. The national security mission has never been more crucial as we face an uncertain world and the new reality that the borders of our nation are not impenetrable. As both Laboratory employees and private citizens, we are reminded daily of the threat posed by rogue states and terrorists and of our duty to serve our nation by ensuring its safety through cutting-edge advances in science and technology.

Each employee of the CMS Directorate is a necessary component of a team that has achieved success and whose continued success is vital to the Laboratory and our country. This team—our team—is charged with extraordinary responsibilities in an environment of continuous change, as explained in the closing section. We have been called on to execute and support the Laboratory's most important programs in national security, homeland security, energy, environment, and health as well as to conduct fundamental research inspired by these programs.

We should all be proud to be part of today's CMS Team. This team will bring both innovation and a sense of resolve to bear on the national security challenges we face. As we continue to strive toward excellence in the chemical and materials sciences, we—the CMS Team—will eagerly anticipate the strengthening of our nation's safety and the advancement of the frontiers of science.

Looking toward our successful future,

Tomás Díaz de la Rubia



CMS is committed to building strong dynamic teams.

CMS Strategic Plan Aligns with the Laboratory's Long-Range Plan for Science and Technology

Sustained investment in science and technology (S&T) ensures the vitality of our Laboratory. Outstanding S&T makes it possible for Livermore to meet the demands of current missions and respond to new challenges to the nation.

This past year, senior Laboratory scientists and managers were tasked by the Director to craft a long-range plan for S&T investments. The plan is intended to provide a mechanism to guide decisions at the Director's level about institutional investments that create new research and development (R&D) opportunities, bolster recruiting, and enhance Livermore's scientific facilities and infrastructure. The plan is also intended to provide employees with a clear view of the strategic directions of the Laboratory.

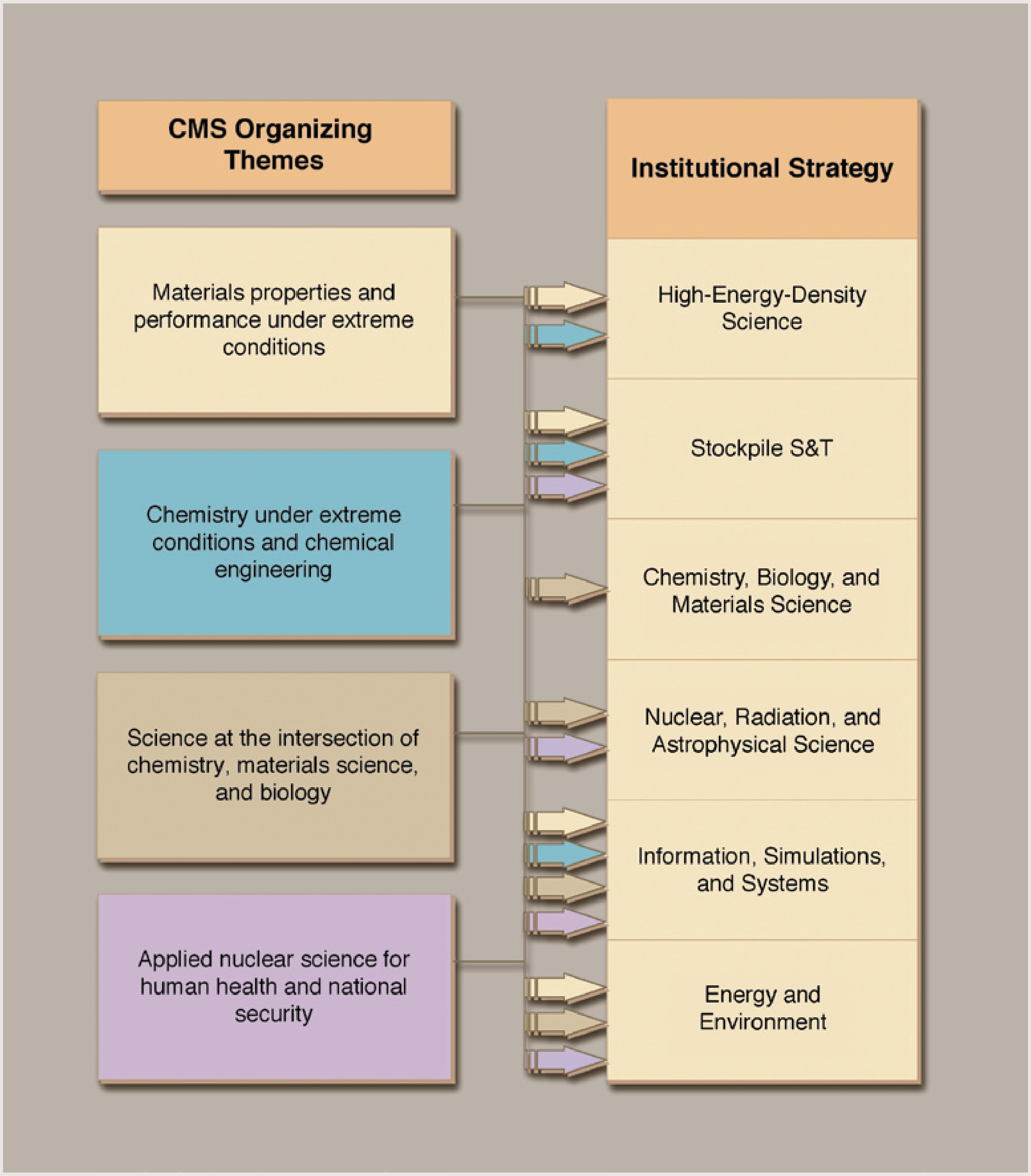
The CMS strategic plan presented in these pages derives from, and is fully synergistic with, the Lab's long-range S&T investment strategy, which has six thematic areas:

- **Stockpile Science and Technology:** Develop novel designer materials through initiatives in nanoscale materials synthesis and provide new real-time, in situ diagnostics for the investigation of the properties and performance of materials under extreme dynamic conditions.
- **High-Energy-Density Science and Technology:** Develop revolutionary radiographic diagnostic capabilities for the National Ignition Facility (NIF), which will greatly enhance NIF's unique contributions to stockpile stewardship, and explore the enormous scientific opportunities in high-energy-density physics that are created by adding an ultrafast, ultra-intense laser capability to NIF.
- **Nuclear, Radiative, and Astrophysical Science and Technology:** Develop better radiation detectors, make major advances in laser-electron-beam science and technology, and explore the physics of unstable nuclei, which will contribute to the Laboratory's national security mission and define a significant role for Livermore in emerging international science projects.
- **Chemical, Biological, and Materials Science and Technology**: Develop a quantitative, predictive understanding of biological phenomena at the molecular and cellular level and apply this knowledge to combat chemical, biological, and radiological threats to national security and to improving our understanding of the fundamental mechanisms of microbial biology.
- **Information, Simulation, and Systems Science and Technology:** Enable insight from the increasingly vast amounts of information generated by simulations, experiments, and intelligence; merge and validate simulation and experimental data to facilitate scientific discovery; and integrate and analyze data from disparate sources to provide actionable information to counter national security threats.

An optical component for the National Ignition Facility is assembled in the Optics Assembly Building.

• **Energy and Environmental Science and Technology:** Make major steps in fusion-energy R&D and pursue an integrated program to develop tools to understand, predict, and better manage ecological systems with the aim of improving capabilities to address international security issues such as water availability, climate change and energy demand, and radioactive and toxic releases.

The figure below provides a schematic of how the four CMS organizing themes map into the Lab's institutional strategy, which includes six S&T investment areas.



Materials Properties and Performance under Extreme Conditions

This research theme focuses on the fundamental investigations of the properties and performance of states of matter under extreme dynamic, environmental, and nano-length-scale conditions, with an emphasis on materials of central interest to Laboratory programs and mission needs.

Vision

To provide a fundamental scientific, experimentally validated capability for predicting the properties and performances of materials under extreme conditions, whether dynamic, environmental, or nano-length-scale. To fulfill this vision, the CMS Directorate will take advantage of partnership opportunities with other Laboratory organizations, with the goal of providing science "ahead" of the programs and developing next-generation capabilities that anticipate future mission needs. Consequently, CMS will sustain and enhance its position of national prominence in the field of materials research.

Strategies for Change

CMS seeks to strengthen existing capabilities and create new strategies to predict and experimentally validate properties and performance of materials in extreme environments. When materials are subjected to extremes of highly nonequilibrium conditions of pressure, temperature, strain, stress, and radiation, unusual and unexpected things happen that are outside the realm of everyday experience. For example, changes can occur in structure and strength to the point where material properties become the very antithesis of the original: malleable metals turn brittle, and inert materials become reactive. Moreover, the properties of nanoscale materials—synthesized with atomic-level precision and control—are often dominated by quantum effects with no analogues in the bulk form, leading to unexpected behavior.

Transformations such as these and others can occur under low-energy-density conditions in which materials strength dominates the dynamic response. Transformations can also occur under high-energy-density conditions such as those in the implosion of an inertial confinement fusion target, the ignition of a nuclear weapon, or the collapse of a star. High-energy-density and low-energy-density conditions are typically dynamic conditions, in which the temporal evolution of the material and its properties are important. Materials properties and performance can also be affected by extreme environments that exist under static conditions, such as those that will exist in the high-level radioactive storage facility at Yucca Mountain in Nevada. Finally, extreme length-scale conditions exist in the world of nanoscience, where the properties and performance of materials synthesized "from the bottom up," atom by atom, are dominated by quantum-confinement

Defining Extreme Dynamic Conditions

The science of materials under extreme dynamic conditions can be classified in terms of strongly driven systems (SDS) and high-energy-density (HED) regimes. In a broad sense, the materials science of SDS is characterized as a regime in which the dynamic response is dominated by a material's strength, and the energy scale is less than 1 electron volt. In this regime, matter is "cold" and stiff. The HED regime is characterized by physical conditions at the confluence of condensed-matter physics and plasma physics, where dynamic response is dominated by a material's hydrodynamic flow, and the energy scale exceeds 1 electron volt. In the HED regime, matter is "warm" and fluid.

effects and characterized by properties that have no correspondence in the bulk at the macroscale.

As part of this vision, CMS is partnering with several directorates including Defense and Nuclear Technologies (DNT), National Ignition Facility (NIF) Programs, Physics and Advanced Technologies (PAT), and Energy and Environment (E&E).

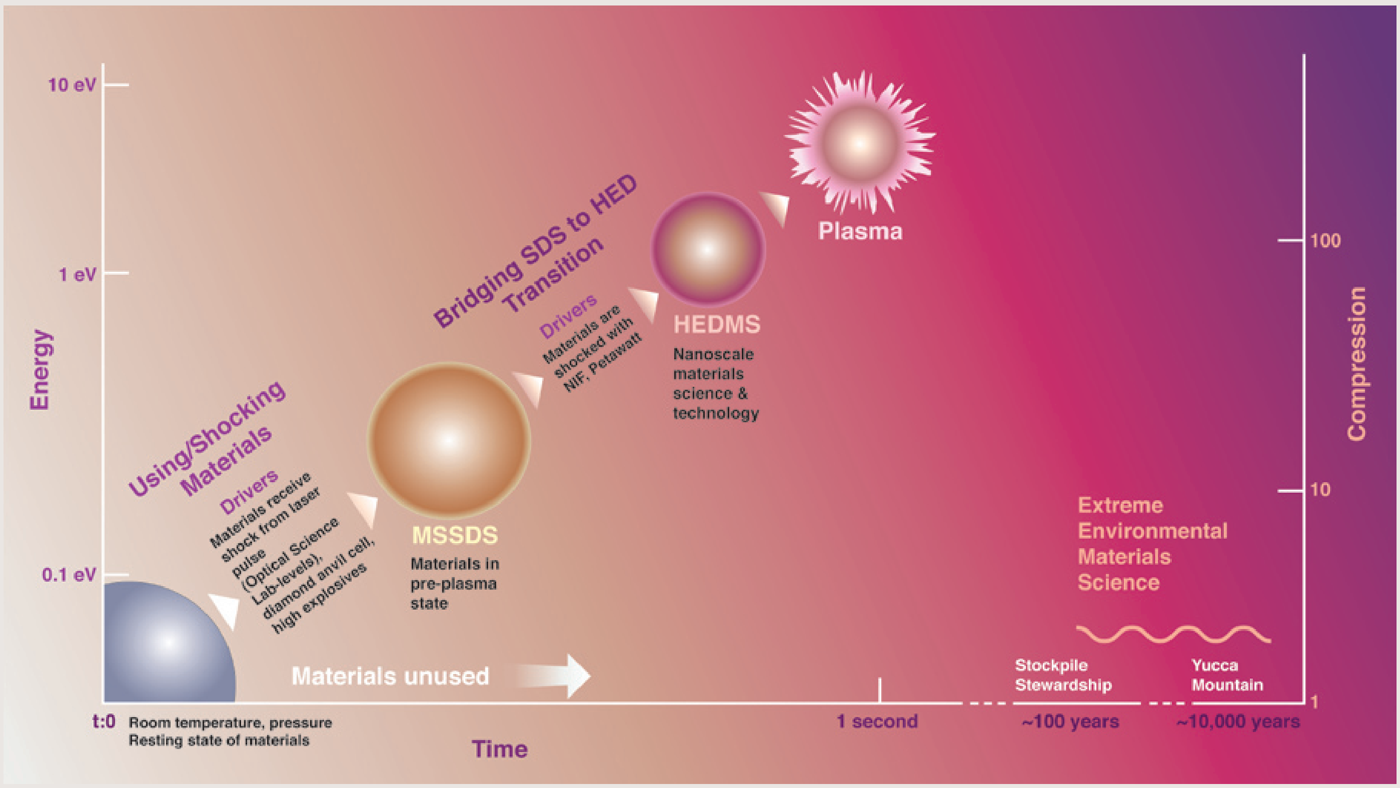
CMS has created strategic objectives for materials properties and performance under extreme conditions in:

• Materials science of strongly driven systems.

• High-energy-density materials science.

• Extreme environmental materials science.

• Nanoscale materials science and technology.



This research theme includes strongly driven systems (SDS), high-energy-density (HED) regimes, nanoscale science, and extreme environmental materials science. Graph of time vs. energy and compression shows general regimes of each of these materials science areas (nanoscience is included in the HED regime).

Materials Science of Strongly Driven Systems

Strategic Objective

Our aim is to provide visionary leadership in establishing an experimentally validated capability for predicting the properties and performance of materials in the low-energy-density regime and to develop real-time, in situ diagnostics that will lead to a truly microscopic understanding of materials properties under low-energy-density conditions.

Materials science of strongly driven systems (SDS) is, at its heart, science for the nation's nuclear stockpile. Resolving important nuclear weapons issues in this regime, such as aging effects on part performance, requires significant advances in fundamental investigations. To this end, CMS plans to extend efforts in areas such as dynamic failure; fracture, spall, and ejecta; constitutive properties, such as strength and plasticity; thermodynamic properties, such as equation of state (EOS) and phase transformation; weapons materials, including metals and alloys; dynamic properties of foams; and plutonium science and technology, particularly ground-state and excited-state properties.

Program Challenges

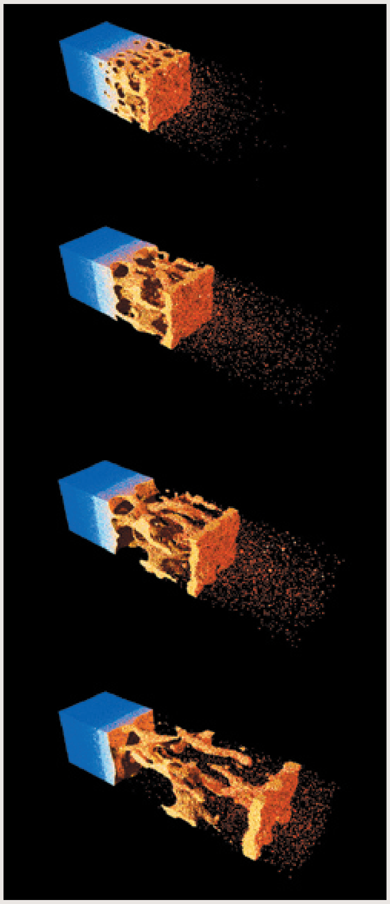
The current U.S. nuclear weapons stockpile consists of a large number of weapons built 15 to 30 years ago. The Stockpile Stewardship Program (SSP) for the U.S. Department of Energy's (DOE's) National Nuclear Security Administration (NNSA) has the goal of indefinitely maintaining this stockpile's viability on the basis of a vigorous and broad-based science program without nuclear testing. Despite SSP's success, central issues remain in developing physics-based predictive models of nuclear weapons performance. Also, the stockpile's advancing age may result in additional refurbishments or unexpected effects that will tax both the scientific and applied functions of the nuclear weapons complex. One key to SSP's continued success lies in improving the fundamental scientific understanding of the complex dynamic behavior in modern weapons, including the dynamic behavior of materials under strongly driven conditions.

Our scientific underpinning for ensuring the performance, safety, and reliability of the stockpile relies on the ability to predict—on the basis of experimentally validated, physics-based models—the dynamic response of materials under a wide range of pressures, temperatures, strains, and strain rates. Without nuclear testing, an understanding of the dynamic responses of materials is imperative because they affect the performance of a baseline design and because they define performance margins and uncertainties over time.

The dynamic response of materials can be broadly described in terms of two classes of properties: thermodynamic properties and mechanical constitutive properties. Thermodynamic properties are determined at the quantum and atomic scales and include EOS, melt, phase transitions, and phase diagrams. Mechanical constitutive properties are governed by phenomena occurring across multilength scales—from atomic to continuum—and are dominated by the collective behavior of defects and the evolution of the material's microstructures. Mechanical constitutive properties include strength, plasticity, fracture, failure, spall, and ejecta.

S&T Challenges

Many science and technology challenges exist in SDS materials science relating to the Laboratory's stockpile stewardship efforts. To meet these challenges, CMS must develop an improved understanding of constitutive properties of plutonium and other materials. New diagnostic techniques must also be developed to study materials under strongly driven conditions. CMS must determine the relationships among materials microstructures, continuum mechanics under extreme conditions, fabrication processes, and failure phenomena such as cracking. A detailed understanding of the physical mechanisms at the microscale will help link those mechanisms to observed results at the continuum scale.



Simulations such as this molecular dynamics model of copper ablation using a femtosecond laser pulse are combined with data from physical experiments to better understand material behavior under extreme conditions.

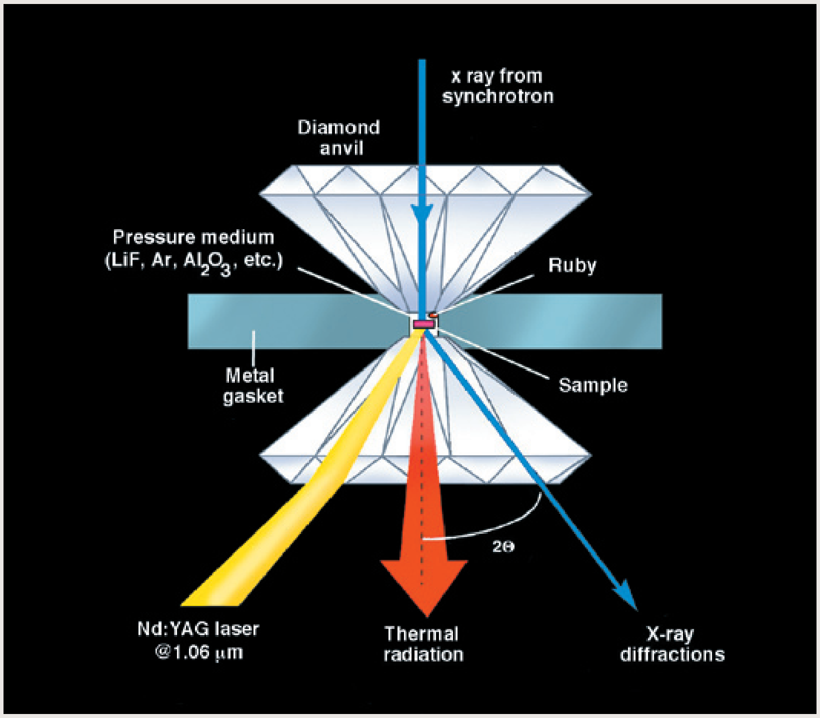
CMS focuses on the following key science and technology elements for developing experimentally validated capabilities to predict the properties and performance on materials under extreme dynamic conditions.

Dynamic shock compression: Investigations of the properties and responses of materials under extreme dynamic compression are central to developing predictive capabilities for assessing the performance and safety of the nuclear stockpile. Experimental facilities and diagnostic capabilities are needed to address issues in EOS, microstructure evolution, dynamic failure and fracture, and materials strength. Executing a broad-based initiative to develop and deploy novel experimental techniques is a high CMS priority.

High-pressure research: A fundamental understanding of the properties of materials under extreme pressure is central to SSP objectives. CMS plans include developing "designer" diamond anvil cells (DACs) to perform in situ measurements, using advanced diagnostics such as ultrabright, fourth-generation synchrotron-radiation sources to obtain measurements of unprecedented accuracy, and integrating static and dynamic high-pressure capabilities by shock loading materials precompressed in a high-pressure DAC.

Actinide science and highly correlated–electron materials: Programmatic needs require that the science of actinides and other f-electron materials (particularly plutonium) be extended to extreme conditions. Three CMS areas in particular need new capabilities and facilities for leveraging real-time results from in situ diagnostics and experiments. The areas of dynamic phase transitions, high-pressure lattice vibrations (phonons) and elastic moduli, and physics of f-electron correlation all afford Livermore researchers unprecedented promise for scientific discovery. (See sidebar on facing page.)

Embedded nanoscale diagnostics: Real-time, in situ diagnostics for development of nanomaterials and nanoscale systems are critical for stockpile stewardship research. For instance, ignition experiments at NIF will require embedded diagnostics with subpicosecond temporal resolutions and fidelity for accurately measuring burn histories, and validation of modern simulation tools require embedded experimental diagnostics that can follow physical processes where and while they happen.



Diamond anvil cells (DACs) capture a sample between an anvil of two diamonds to study materials properties at high pressures and temperatures. The laser-heated DAC technique, shown above, can generate temperatures and pressures experienced in the interiors of the Earth and the Jovian planets, in energetic detonation, and in metallic hydrogen.

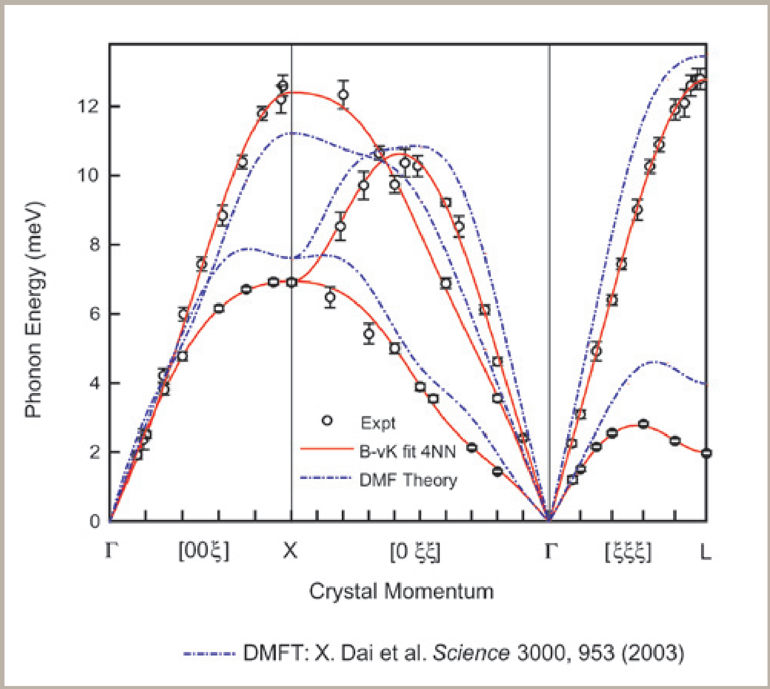
Actinide Science and Highly Correlated–Electron Materials

Plutonium's technological importance stems from the element's nuclear properties: it is highly radiotoxic, emitting alpha particles, and because it fissions with thermal neutrons, it is used in nuclear weapons. However, its place in the periodic table leads to extraordinary electronic properties that still defy a clear explanation, 60 years after they were first discovered. During the last five years, CMS has been co-investing with the DNT program to reenergize experimental plutonium solid-state science and metallurgy. This investment ensures a robust research component to establish the fundamental properties of the most complex metal known.

Investments since 1999 have led to many new insights in diverse areas of plutonium science. They include radiation damage effects observed in the transmission electron microscope, phase stability studied with x-ray absorption fine-structure, and electronic structure measured with conductivity and photoemission spectroscopy. The experimental key to accessing the long-sought-after phonon dispersion curves was developed in an experiment at the European Synchrotron Radiation Facility led by an LLNL scientist, where high-resolution x-ray scattering was used to map, for the first time, the full phonon dispersion.

That the phonons in plutonium would be interesting is ensured both by its place in the periodic table and by experiments performed many years ago. These measurements showed that the elastic properties of fcc plutonium are highly direction dependent (anisotropic). Ever since, the field has waited to learn more of the properties of plutonium, particularly its elementary excitations at finite q (a parameter that is inversely proportional to the wavelength of the excitation). A recent experimental study by a CMS researcher and an international research team has elucidated the elementary transitions (the movement of atoms in the solid), an aspect of plutonium that has not been experimentally addressed before and that provides unique laboratory validation for complex materials codes.

This "front-end" of plutonium science is the foundation and logical starting point for the extension of this same science to dynamic dimensions. High-resolution electron spectroscopy, using ultrabright electron beams and synchrotron light; physical property measurements as a function of composition, field, and pressure; and the metal physics of defects and interfaces, are all experimental and theoretical areas of continuous investment that will ensure success in the expanding frontier of the dynamic properties of actinide and highly correlated–electron materials.



The agreement between modern many-body electron theory (blue lines) and experiment is surprisingly good. However, a noticeable difference appears in the [111] direction, especially at short wavelengths. This feature probably arises from the electron–phonon interaction. A natural extension is to follow such effects as a function of composition, temperature, and pressure.

High-Energy-Density Materials Science

Strategic Objective

By providing insightful leadership to the Laboratory's growing high-energy-density materials research, CMS will extend experimental and simulation capabilities, particularly in the areas of warm dense matter; low-temperature, solid-density plasmas; and dynamic properties of low-Z foams required for targets for world-class, high-energy-density platforms such as NIF, Omega, and the next-generation petawatt lasers.

High-energy-density (HED) materials science explores the behavior of materials in regimes found in the center of a star and in the heart of an exploding nuclear weapon. Experiments on NIF at Livermore will allow access to previously unattainable HED regimes. To meet the challenges of this new and exciting field, CMS must extend its experimental and simulation capabilities in the science of HED materials. Of particular importance is the development of predictive capabilities to describe the properties of matter in the warm dense matter regime overlapping condensed matter and plasma physics. This capability will afford CMS unparalleled opportunities for discovery-class science.

Program Challenges

Livermore has a long-term investment strategy in long-pulse HED science through laser facilities such as NIF and Janus at Livermore, Omega at the Laboratory for Laser Energetics at the University of Rochester, Helen at the UK Atomic Weapons Establishment, and the Rutherford Appleton Laboratory's Vulcan laser system in the UK. Moreover, Livermore facilities such as the ultrashort pulse laser facility present scientific opportunities for creating warm states of matter and interrogating dynamic response in the ultrafast regime. The Laboratory's focus on HED provides CMS with partnerships with DNT, PAT, and NIF.

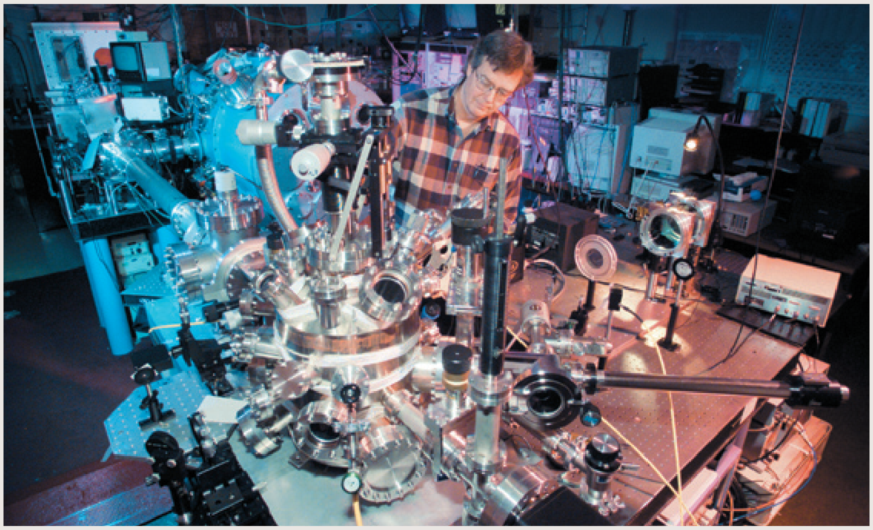
Short-pulse, high-intensity lasers are important tools for HED materials research. These lasers provide methods for creating ultraHED plasma sources that directly match the conditions found in stars and nuclear weapons. They can also probe phase transitions and their kinetics on timescales that approach the intrinsic timescales for material response. New capabilities include intense, energetic particle beams for rapid heating of materials; high-temperature, high-energy proton beams for radiography with high space and time resolution; and picosecond x-ray lasers for interferometry and high-density material probes. NIF, in combination with the Advanced Radiography Capability, will greatly extend laser capabilities. The creation and direct probing of HED materials conditions will be possible in the laboratory. HEPW laser-generated particle beams or radiation sources will allow interrogation of extreme states of temperature and pressure on picosecond timescales.

The creation of HED conditions in the laboratory has important scientific ramifications that complement some of the challenges facing Livermore's stockpile stewardship effort.

S&T Challenges

Opportunity is beckoning for Livermore to invent a new field of HED materials science and become its research leader. We are committed to advancing several principal science and technology challenges: warm dense matter (WDM); low-temperature, solid-density plasmas; and dynamic properties of low-*Z* foams used in HED targets. Other challenges exist in developing ultrafast in situ probes and methods to investigate ultrafast dynamics.

WDM is at the confluence of the traditional fields of condensed matter physics and plasma physics. However, neither solid-state band theory nor



Adjusting sample position on the electron time-of-flight (eToF) spectrometer used for time-resolved, pump-probe experiments on the COMET x-ray laser.

ideal gas plasma theory applies. In addition, EOS and transport models are theoretically intractable, leading to large uncertainties for EOS and opacity models important in astrophysics.

In close collaboration with the PAT, DNT, and NIF directorates, CMS plans to target investments in key WDM areas: theory, high-performance computing and simulation, experiments, and advanced in situ diagnostics.

For modeling and simulation, our objective is to extend conventional electronic structure methods and approaches to finite-temperature treatments of the dynamic behavior of WDM states—including the treatment of electronic excitations and structural phase transformations.

For experiments and advanced real-time, in situ diagnostics, advanced experimental pump-probe experimental methods will be deployed using intense, high-brightness, fourth-generation synchrotron radiation sources—the Sub-Picosecond Photon Source (SPPS) and the Linac Coherent Light Source (LCLS)—with high-intensity lasers.

CMS will also exploit third-generation synchrotron radiation sources, such as the Advanced Photon Source (APS) and the Advanced Light Source (ALS), which are key experimental facilities investigating properties of matter under extreme conditions. In addition, CMS is leading a research effort to investigate the electronic response of materials subjected to high temperatures, as produced by the COMET x-ray laser operated by the PAT Directorate.

Ultrafast in situ probes for materials and plasma dynamics will provide key tools to stockpile stewardship researchers who need highly accurate understanding of EOS and dynamics at high pressure. The sources and techniques developed for such probes could also be used by other high-pressure facilities. (See sidebar.)

Ultrafast Diagnostics for Materials Dynamics

The recent explosion of pump-probe studies into the picosecond time-dependence of chemical reactions has been based largely on laser pump and laser or synchrotron radiation interrogation techniques. The observation of intermediate metastable states in phase transformations, chemistry, and biology is of particular interest for gaining insight to reaction pathways. Much less attention has been given to approaches based on laser-induced and electron-interrogation methods, despite the fact that electron sources are brighter and their interactions with matter stronger.

The small but rapidly developing field of pump-probe ultrafast electron diffraction (UED) uses pulsed instruments with ~500-femtosecond time resolution. They often include a laser to drive the sample before electron probing. A similar effort in nanosecond imaging in the transmission electron microscope (TEM) has been ongoing at the Technishe Universität Berlin for the last decade. The dynamic transmission electron microscope (DTEM) is a newly developed technique that combines all of the powerful techniques of the standard TEM with nanosecond time resolution for capturing dynamic processes while they occur. Images with high spatial resolution (~1nm) can be acquired that will show the salient features of materials microstructure, such as dislocations, impurities, grain boundaries, and phase boundaries. The technique has also been demonstrated with the acquisition of multiple frames, with spacings in time from 10 ns to several 100s of ns. Multiple frames allow the evolution of a dynamic process to be followed. The high time resolution on the microscope is achieved by creating a short pulsed, intense source of electrons that are used to illuminate the specimen and expose the CCD recording device. At LLNL, we are developing both an ultrafast electron microscope and an ultrafast electron diffraction instrument intended for the study of complex transient phenomena with unprecedented spatial and temporal resolution.

CMS is actively pursuing ultrafast electron-based diagnostics—both UED and DTEM—for real-time, in situ probing of the atomic-level response of materials. Key applications include structural phase transformations, shock-induced melting, and dynamic failure. Moreover, CMS is engaged in an LDRD-supported Strategic Initiative on real-time, in situ measurements of the dynamic response of materials under laser-driven shock loading conditions. The core scientific objective of this SI is to interrogate "on the fly"—on the basis of electron and photon probes—the dynamic response of the material at the atomic-level and to develop a scientific basis to link this atomic-level response to continuum observables.

Nanoscale Materials Science

Strategic Objective

We will provide unparalleled leadership in the area of nanoscale materials synthesis, characterization, and high-performance modeling and simulation in alignment with the Laboratory's mission needs in national security, inertial confinement fusion, and energy and environment.

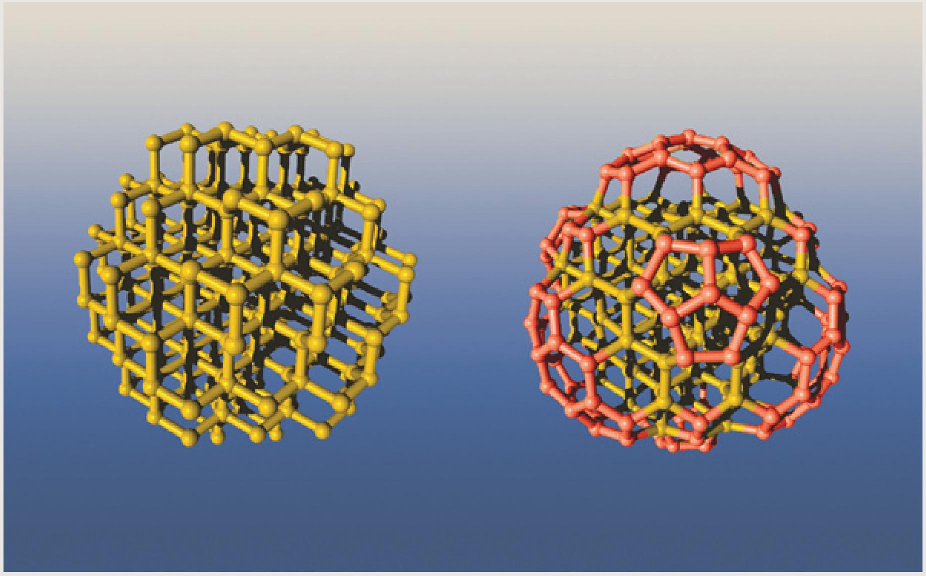
Nanotechnology is the creation and use of materials, devices, and systems through the control of matter on the nanometer-length scale (at the level of atoms, molecules, and supramolecular structures). Nanostructures, made with building blocks whose properties can be predicted from first principles, exhibit novel physical, chemical, and biological properties and phenomena. Livermore aims to enhance current capabilities and develop new ones in nanotechnology and to exploit their properties for future efficient manufacturing and use of these structures as needed by Laboratory missions.

Materials with nanoscale features often have properties and performance that are dominated by quantum confinement and other effects and exhibit properties without analog at the macroscale. CMS focuses on the synthesis of these materials and in the identification of their characteristics, an effort referred to as nanoscale synthesis and characterization. For example, by controlling the exact composition of materials at the nanoscale, CMS researchers will be able to precisely control an object's structure and predict with confidence how the object will behave under extreme dynamic conditions.

Other applications of nanoscale materials science include the synthesis of sensors and detectors whose properties can provide signatures to biological and chemical agents. Important aspects of nanoscale materials science are our ability to model—at the quantum and atomic scales—and predict the properties and response of nanostructured materials on the basis of high-performance simulation tools. Our quantum-and atomic-level materials simulations are particularly well suited to guide experiments involving nanostructured materials because the scale of the simulation (atomic) is commensurate with the natural length scale of the structure whose properties are being investigated. Nanoscale materials science offers a striking example of experiments performed at the same length scale as those afforded by high-performance atomic-level simulations.

Program Challenges

The Laboratory's long-range plan for stockpile science and technology identifies as its primary objective the quantification of margins and uncertainties in nuclear weapons performance. Nanoscale materials science and technology will help quantify these uncertainties. For example, the targets fabricated and assembled for stockpile science experiments on NIF and other platforms must be diagnosed with penetrating probes, so that researchers can "see" in real time physical phenomena occurring on the scales of picoseconds and hundreds of nanometers. The information gathered will lead to a high-fidelity understanding of key complex physical processes. Other stockpile science applications include radiation transport, complex hydrodynamics, EOS, and opacity. In addition, nanoscale materials science is key to the development of specialized sensors and detectors that have properties tailored for specific applications. The Laboratory has launched the Nanoscale Synthesis and Characterization Laboratory (NSCL) to serve as an institutional incubator, supporting Livermore's missions in national security, inertial confinement fusion, and energy and environment. (See sidebar on p.14.)



In first-principles simulations of nanodiamond, the surface of a 1.4-nanometer nanodiamond (left) with 275 atoms spontaneously rearranges itself into a fullerene (right) at about 300 kelvins.

S&T Challenges

The science and technology challenges are many:

• Predictive capabilities for structure–property relationships at the nanoscale level.

• Atomic-scale control of interfaces and surfaces.

• Atomic-scale control of mechanical properties.

• Molecular-scale control of chemical reactivity.

• Nanoscale machining and characterization fundamentals.

• Metrology of physically and chemically complex structures.

• Precision micro-assembly.

• High-performance computational materials science and chemistry.

Laboratory capabilities supporting these challenges include:

• Equipment to synthesize and characterize materials and prototypes.

• Synthesis tools.

• Metrology.

• Nanomechanics.

• Analytical capabilities.

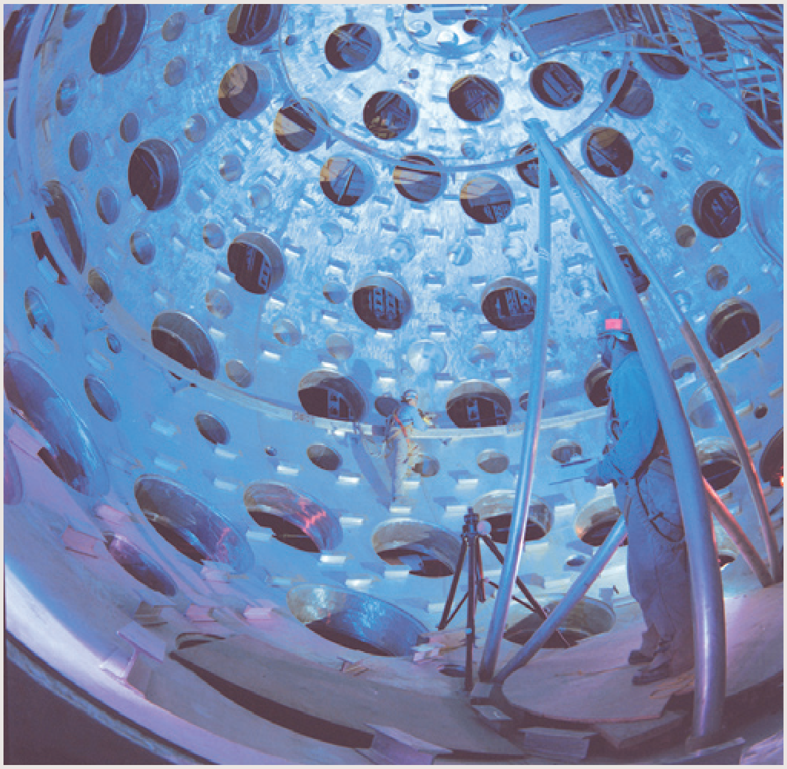
• Modeling and analysis.

• High-performance computing platforms.

The synthesis and characterization of targets for HED science experiments is a significant initial focus of the NSCL. HED targets for NIF are complex, multilayered physical and chemical structures with dimensions ranging from microns to millimeters, requiring precise assembly of micron-sized pieces. Among the challenges are the tailored creation and understanding of metal foams, bonding and joining, and enhanced characterization of nanoscale materials properties.

Metal foams will have uses in ablators (where the laser energy or x rays are absorbed), pushers (which apply hydrodynamic pressure to inner layers), backlighters, and hohlraums. At the cell sizes required, surface and interface atoms will make up several percent of the total atoms in the material, as opposed to bulk materials in which surface atoms make up only one part in ten million. Research on these foams will enable control of surface and interface properties. Understanding the surface properties will help address issues such as creep, in which a metal foam moves much like window glass over time.

CMS must find new ways to join or bond the materials that make up these targets, to better match simulation models. In a key effort, we hope to find an intermediate solution using molecular-scale linkages that approach the zero thickness of the bonding layer in simulations. We will also study the use of precision sculpting, in which the surface perturbations created vary from submicron in amplitude to many microns in period.



Workers are dwarfed inside the 10-meter-diameter NIF target chamber. One challenge is to fabricate and assemble complex millimeter-sized targets for stockpile stewardship and other experiments that will be conducted in this chamber.

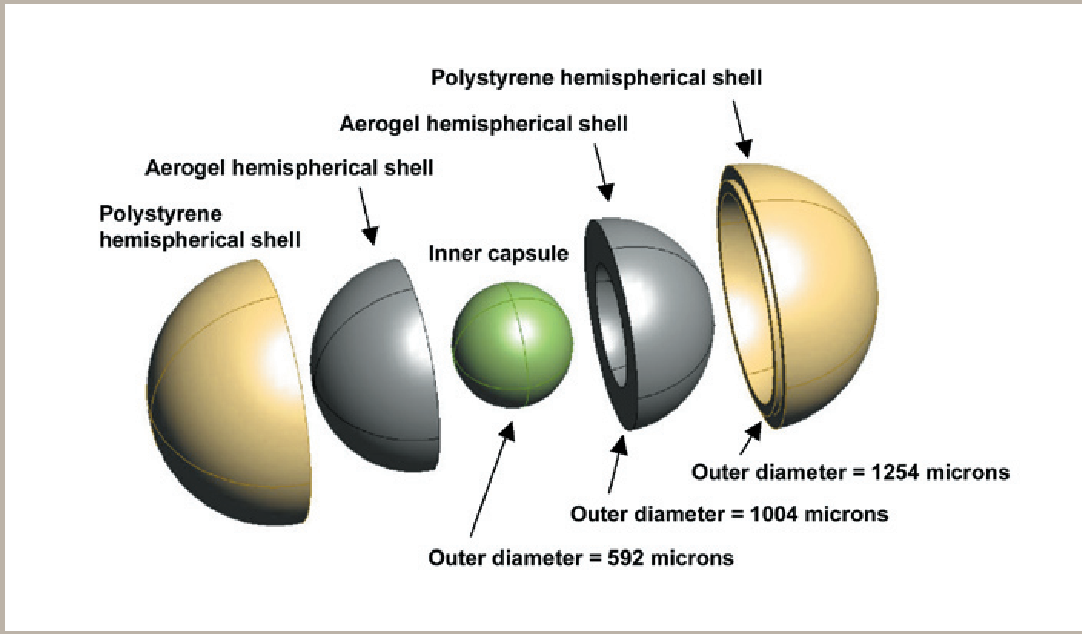
Nanoscale Synthesis and Characterization Laboratory

One result of the Laboratory-wide strategic planning exercise was the identification of designer materials as a stockpile science "sweet spot," that is, an area where an incremental investment would have a large benefit. CMS, in partnership with Engineering, created the Nanoscale Synthesis and Characterization Laboratory (NSCL) to focus institutional science and technology investments on materials that advance stockpile stewardship.

The NSCL's primary mission is to create and exploit interdisciplinary research and development opportunities in nanoscience and technology. Advances in nanoscience and technology will result in new materials, fabrication processes, structure assemblies, and characterization methods that will benefit LLNL's mission. The NSCL will showcase the application of interdisciplinary team science to solving important national problems. Projects are expected to range from the development of monolayer chemical links to foam casting. The NSCL will also recruit and train personnel for Livermore programs in DNT, NIF, and NAI and will partner with academic research centers.

The NSCL investments are a strategy to lead stockpile science to new materials solutions. There are three primary areas of focus for early NSCL efforts. The initial focus is in target science for HED experimental platforms such as the NIF, Omega, and Janus lasers and the gas guns. Research on nanoporous and gradient density materials is critical to this work. The second focus is establishing abrupt interfaces between similar and dissimilar materials, nanoporous and nonporous materials. Finally, the NSCL will develop high-strength nanocrystalline materials for target capsules.

The target science and technology capabilities of the NSCL are being deployed in support of an LDRD-supported Strategic Initiative on double-shell target research and development for noncryogenic "fast-track" ignition on NIF. The objective of this SI is to integrate advanced design concepts, experiments on pre-NIF facilities, and materials science development for target fabrication.



The NSCL is developing advanced nanoscale materials synthesis and characterization capabilities for the fabrication of double-shell, noncryogenic targets for ignition on NIF.

Strategic Objective

By providing leadership to the Laboratory's growing emphasis on extreme-environment materials research, the CMS Directorate will extend experimental and simulation capabilities, particularly those supporting the investigation of material degradation and the enhancement of related fabrication processes, as well as next-generation corrosion-resistant materials and beneficial uses of nickel and depleted uranium.

Extreme-environment materials science can be viewed as an extension of SDS materials science, with the focus on predicting the response of materials to extreme environments over 10,000 years. Such environments are characterized by high ambient temperatures (up to 150°C) and high radiation levels (up to 180 rad per hour) in the presence of corrosive agents. Long-term prediction is challenging because of the great discrepancy between the timescale of experiments and predictions. To meet this challenge, CMS must extend experimental and simulation capabilities in the area of slow but sustained reactions under environmentally severe conditions. Among the areas amenable to computer simulation are thermodynamics of mineral solutions in water, stability of alloys over very long times at moderately low temperatures, corrosion of metals, stress corrosion, and hydrogen-induced cracking.

Program Challenges

The challenge of extreme environmental conditions over extremely long time spans is the province of DOE's Yucca Mountain Project (YMP). The project's goal is to create a safe, long-term geologic repository for the permanent disposal of both spent nuclear fuel from nuclear power plants and high-level radioactive waste from nuclear weapons production.

Although Livermore involvement in the project dates to 1977, our current focus is on developing a system of engineered barriers surrounded by natural barriers to contain the highly radioactive waste. Little is known about how modern materials, placed in a geologic site and subjected to initially high temperatures and radiation, will behave during such time periods. Thus, much of Livermore's development work is based on predictive models and accelerated age testing of materials and systems. The engineered barrier system (EBS) includes the containers that will hold the waste and a complex series of interactions of the waste and packaging with the immediate or near-field environment.

Most major materials issues facing YMP involve a nickel–chromium–molybdenum alloy (Alloy 22), which will form the outer barrier of the EBS waste package. Programmatic challenges for CMS technical leadership include determining the long-term metallurgical stability of alloys under radiation, determining the long-term integrity of Alloy 22 welds and exploring alternative welding processes, and reducing uncertainties in current models of corrosion behavior in Alloy 22.

CMS must continue efforts to reduce major uncertainties existing in the long-term values of the corrosion potential used in computer models. Experimental data and analytical modeling regarding tensile stresses on the waste packages are also insufficient. Theoretical and

The Yucca Mountain Project includes research on an engineered barrier system. The system will contain radioactive waste deep underground and 300 meters above groundwater and must last at least 10,000 years under varying and extreme conditions of temperature, radiation, and corrosion.

experimental studies of crack-arrest mechanisms and probability would enhance the Laboratory's research on long-term crack initiation. Finally, the family of alloys that includes Alloy 22 is susceptible to hydrogen embrittlement, which weakens the alloy. We need a better overall understanding of how variables such as alloy composition, cold working, and thermal history interact to affect susceptibility.

S&T Challenges

The S&T challenges facing the Yucca Mountain Project bring a unique opportunity to Livermore researchers. The solution will be leveraged from work under way in SDS materials science for stockpile stewardship and highly enriched uranium transparency. Specific, significant challenges include developing a fundamental understanding of metal alloy stability over extremely long time periods and of the different types of corrosion phenomena. Another challenge involves obtaining a theoretical understanding of the hydrogen embrittlement phenomenon at very small rates over very long time periods. CMS researchers also must develop a thorough understanding of gamma radiolysis of environmental agents in the gas/liquid phase as well as in surface films, new techniques for remotely interrogating materials, and analytical techniques to detect extremely low levels of radioactive contaminants in groundwater.

To address these challenges, CMS must develop new capabilities or extend current ones in the areas of thermodynamics of metal alloys and theoretical mechanistic understanding of corrosion of metals. CMS must also explore the kinetics and effects of hydrogen embrittlement over long time periods, develop phenomenological models of stress corrosion cracking and crack stifling mechanisms, and develop a theoretical understanding of laser peening. Finally, the current integrated phenomenological model of the Yucca Mountain Repository must be enhanced to include all physicochemical processes including the fate and reactive transport of gas, droplets, and films into the emplacement drifts.

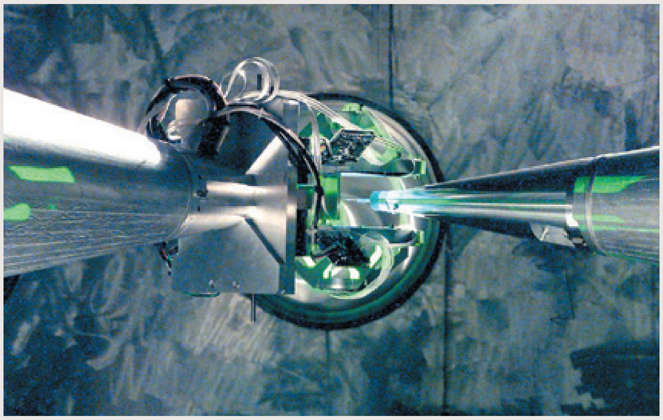
Crosscutting Issues

By its very nature, the fundamental investigation of the properties and performance of materials under extreme conditions cuts across several programmatic and disciplinary organizations at the Laboratory. Consequently, unique opportunities for leverage and partnerships stretch across three technical areas: theory, modeling, and simulations; dynamic experiments using advanced real-time, in situ diagnostics; and nanoscale materials science and technology.

Theory, modeling, and simulations: The challenge will be to integrate condensed matter physics approaches with plasma physics formalisms to predict the properties and performance of states of matter subjected to extreme dynamic conditions. In particular, the plasma physics treatments of hot dense states of matter could lead to incorporating finite-temperature effects in computational condensed matter and materials physics applications. In the area of nanoscale materials science, modeling will be needed for producing the new synthesis parameters to reach the design requirements for HED targets.

Dynamic experiments and in situ diagnostics: Experimental capabilities will be bridged to facilities (e.g., specially instrumented diamond anvil cells, two-stage mechanical launchers, high-energy laser platforms) that provide complementary capabilities for various regimes. Crosscutting technologies for advanced real-time, in situ diagnostics also exist, particularly for interrogating atomic-level dynamic response of materials under shock loading conditions. These technologies include advanced radiography, optical (VISAR) diagnostics, and dynamic x-ray diffraction.

Nanoscale materials science and technology: Several directorates are involved in crosscutting activities including atomic-level synthesis and characterization of low-dimensionality materials, micro-assembly of experimental targets, and high-performance modeling and simulation to design and predict the properties and response of materials with nanoscale features. The NSCL will integrate and coordinate these activities for timely advances in the field that will, in turn, enable the Laboratory to be recognized as a significant contributor.



A look inside the NIF target chamber.

Workforce Requirements

The future workforce and leadership for extreme materials science will be drawn from several disciplines including condensed matter physics and materials science, plasma and atomic physics, shock physics, high-pressure research, laboratory astrophysics, and optical and laser science. The Laboratory must attract, retain, develop, and nurture next-generation leadership in this critical area.

CMS must grow the next generation of materials scientists in nontraditional fields such as warm dense matter physics and HED materials physics. People are also needed who have the theory and simulation skills to bridge microstructure, engineering, and design codes. CMS must recruit and retain people with skills in dynamic experiments on SDS and HED experimental platforms as well. More specialists such as actinide metallurgists and chemists are needed as well as a large technical support contingent.

Because of the requirements of NNSA and DOE, the proportion of U.S. citizens must be increased. Challenges lie in attracting and retaining a workforce with the requisite expertise. For example, university training for plutonium metallurgists is nonexistent and nearly so for plutonium and nuclear chemists. The dearth of such experts will affect recruitment efforts.

CMS must also bring in subject experts in nanoscale synthesis and joining. The Nanoscale Synthesis and Characterization Laboratory will be the principal draw in attracting, recruiting, and retaining these specialists.

The long-term nature of the Laboratory's national security mission, particularly in stockpile stewardship, makes attraction and retention of the best and the brightest staff a critical strategic element of this plan. Although there are significant tactical reasons for involving university collaborators and their students in current research programs, even more leverage will be gained in the long term. For example, some of the graduate students and postdocs now working on NIF will become principal investigators, innovators, and program leaders, developing and executing experiments only dreamt about today.

The Laboratory has a long-term commitment and obligation to the Yucca Mountain Project. Consequently, CMS must develop and maintain a cadre of researchers with relevant specialties in, for instance, radiolysis by gamma rays, computational thermodynamics and phase kinetics of alloy systems, and understanding of the effects of laser peening process on corrosion behavior. In addition, CMS must attract modelers and systems engineers who can integrate those phenomena and develop a coherent model of the repository for confidently predicting materials performance.

CMS should build a focused strategy around its postdoc programs, fellowships, and graduate students with the stockpile stewardship mission in mind. Summer schools and workshops are excellent venues for emphasizing our scientific vision. Finally, Livermore and NNSA are making significant investments in university research under the aegis of the Advanced Strategic Computing (ASC) University Alliance and NNSA Academic Alliances. CMS must ensure that participants have significant collaborations with and mentoring from LLNL scientists and engineers.

CMS must attract people with strengths in a variety of areas—from dynamic experiments on HED platforms to experts in nanoscale synthesis—to address the challenges of the future.

Infrastructure Requirements

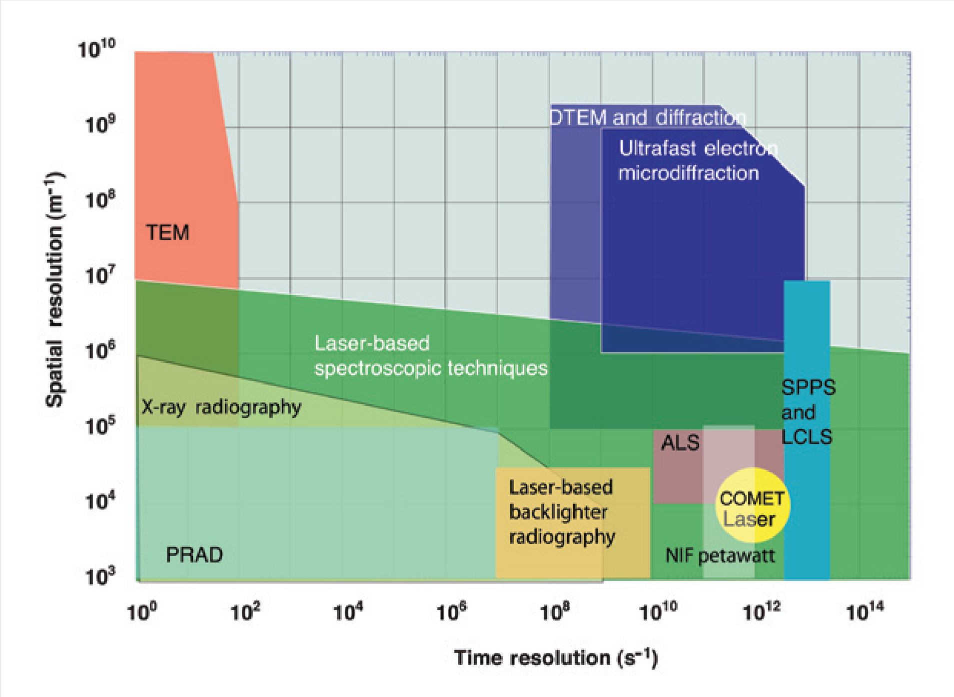
The primary infrastructure requirement is the integrated "signature" facility: The Center for Extreme Materials Science and Chemistry. This center will provide a focus for many activities described herein and for the necessary capabilities and expertise. Experimental capabilities required include heated, instrumented DACs; two-stage mechanical launchers; *Z*-pinch accelerators; high-energy laser platforms; and synchrotron-radiation user facilities. Also, CMS will leverage infrastructure requirements for SDS and HED materials sciences, given that the two require a similar set of dynamic experimental facilities. In particular, CMS will make extensive use of the unique capabilities afforded by national synchrotron-radiation user facilities, including third-generation (ALS, APS) and fourth-generation (SPPS, LCLS) light sources.

For SDS experiments, CMS must invest in diagnostics such as ultrafast x-ray detectors, intense fast portable probes, and ultrafast electron microscopy capabilities. More "agile" lab space—offering improved diagnostics for temperature, pressure, and surface velocity—is needed, including more small-sample facilities operating at the radiological level. Cost, time, and workforce considerations affect these requirements. The cost of developing and executing plutonium operations, for instance, is rising fast, and new experiments come on line slowly. If a new glovebox can take years from design to operation, new facilities can take decades. Capturing and keeping high-quality scientists for these efforts will be nearly impossible.

For HED materials science, CMS must ensure that diagnostic support for short-, mid-, and long-term integrated experimental teams is properly integrated for HED materials dynamics experiments on NIF.

For nanoscale materials science, CMS must invest in the Nanoscale Synthesis and Characterization Laboratory and systems such as the focused ion beam (with an add-on for x-ray tomography), a nanoindentor, an x-ray source, and a nanoscale assembly station for research and prototyping.

For extreme-environment chemistry, needs focus on materials degradation and life prediction for the YMP. For instance, tools are needed to characterize materials' oxide surface structure, composition, and stress state. Techniques are needed for in situ monitoring of corrosion processes and for understanding the chemical evolution (including biological effects) of thin aqueous films.



CMS is making strategic infrastructure investments in the area of ultrafast electron-based diagnostics, including ultrafast electron diffraction (UED) and dynamic transmission electron microscopy (DTEM). Electron-based probes afford unprecedented time and spatial resolution to investigate ultrafast phenomena in materials, and chemical and biological systems.

Chemistry under Extreme Conditions and Chemical Engineering

This research theme focuses on investigating the chemical properties, reactivity, synthesis, and engineering of energetic, optical, and other high-performance materials under ambient equilibrium and "extreme" nonclassical conditions that arise during dynamic shock-, temperature-, and radiation-induced transformations.

Vision

To establish excellent discipline-based science and technology in the fields of chemistry under extreme conditions and advanced materials synthesis and chemical engineering while simultaneously providing key programmatic support to the Laboratory in the areas of energetic materials (e.g., explosives, propellants, and pyrotechnics), optical materials, and chemical detection and process engineering.

Strategies for Change

To fulfill this vision, the Chemistry and Materials Science (CMS) Directorate will lead development of new science and technology R&D that anticipates programmatic needs at Lawrence Livermore National Laboratory (LLNL). A long-term stable commitment to vision goals will help ensure success. Collaborations with National Nuclear Security Administration (NNSA) centers, universities, private labs, and Department of Energy (DOE) facilities will continue to reinvigorate our directorate by providing fresh ideas and talented young scientists. During the next five years, we will set the course that puts Livermore at the forefront of virtually untouched fields of chemistry and engineering.

Directorate capabilities in key strategic areas—energetic materials, materials compatibility and aging, synthesis of new materials, laser optics and target fabrication, computational chemistry, and hydrodynamic modeling—are helping advance core Laboratory missions. These mission areas range from advanced conventional weapons to stockpile stewardship, from the forensics of weapons of mass destruction to the technical challenges of homeland security.

Through several research collaborations, the directorate is working to advance understanding of the combustion and energy-release mechanisms of energetic materials and nanocomposites. By advancing understanding of these mechanisms, CMS seeks to position the Laboratory to reap the full potential of energetic nanomaterials. (See sidebar to right.)

CMS is also seeking to enhance understanding of the response of energetic materials to various stimuli through an interdisciplinary approach that combines experimental studies using different length scales, from nanometers to meters. Furthermore, by enhancing our capabilities, we will help meet the need of Laboratory

Energetic Nanomaterials

At the Laboratory, sol-gel chemistry—the same process used to make aerogels or "frozen smoke"—has proven to be key in creating energetic materials with improved, exceptional, or entirely new properties. A team of researchers in the Energetic Materials Center engineered this breakthrough. Using sol-gel processing methods, the team derived four classes of energetic materials: energetic nanocomposites, energetic nanocrystalline materials, energetic powder-entrained materials, and energetic skeletal materials. These new materials have structures that can be controlled on the nanometer (billionth-of-a-meter) scale. In general, the smaller the size of the materials being combined, the better the properties of energetic materials.

Because these nanostructures are formed with particles at the nanometer scale, their performance can be improved over materials having particles the size of grains of sand or powdered sugar. In addition, nanocomposite materials can be made more easily and safely than materials made by traditional methods.

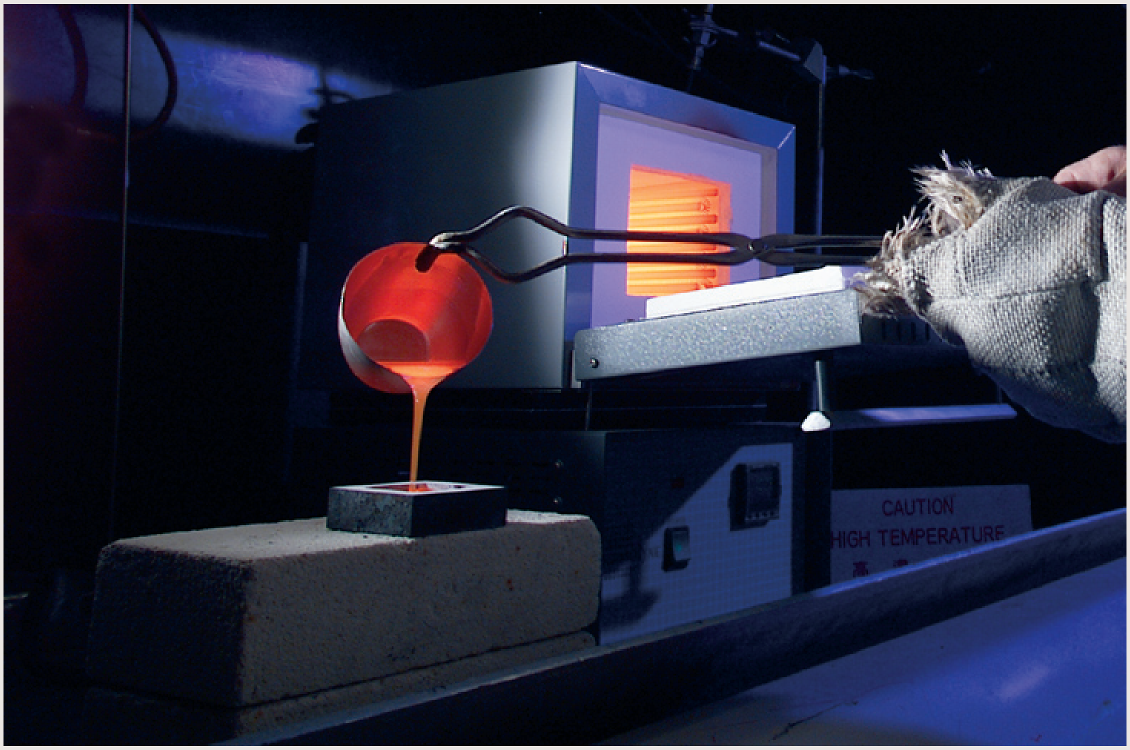
programs to more fully comprehend dynamic chemical processes at high temperatures and pressures.

CMS wants to develop a strong basic science program. CMS believes the program is worth pursuing although difficult at this time because money for basic science is very limited. We must fully understand fundamental issues that govern the safety and performance of our national defense systems, unlock biochemical processes, understand solid-state nanoparticle chemistry, and augment homeland security agendas with our expertise and advanced tools. For example, there is a tremendous scientific opportunity to pioneer basic scientific work in fundamental chemistry at pressures above 1 kilobar with direct application to the Laboratory's core missions and to challenges in geochemistry and astrochemistry.

In addition to improving and sustaining current capabilities needed to support Livermore programs, CMS intends to take the lead for future R&D involving chemistry at extreme conditions of temperature and pressure and to increase the interactions and liaisons with other Laboratory organizations. Primary liaisons are with Defense and Nuclear Technologies (DNT), Homeland Security, National Ignition Facility (NIF), Biology and Biotechnology Research (BBRP), and Energy and Environmental Sciences (E&E).

In creating this strategic plan, CMS has established strategic objectives in two principal thrust areas:

- Chemistry under extreme conditions.
- Advanced materials synthesis and chemical engineering.



CMS personnel with expertise in advanced materials synthesis have been addressing issues of high-temperature glass melting, one of the key technologies applied to NIF optics.

Chemistry under Extreme Conditions

Strategic Objective

We aim to begin a multidisciplinary initiative that will provide, for the first time, a detailed understanding of chemical reaction processes and transition-state chemistry under conditions of extreme pressure (to more than 100 gigapascals) and temperature (to 4000 kelvins). This initiative will enable scientific breakthroughs in several fields and help Livermore programs meet the challenges of national security in the twenty-first century.

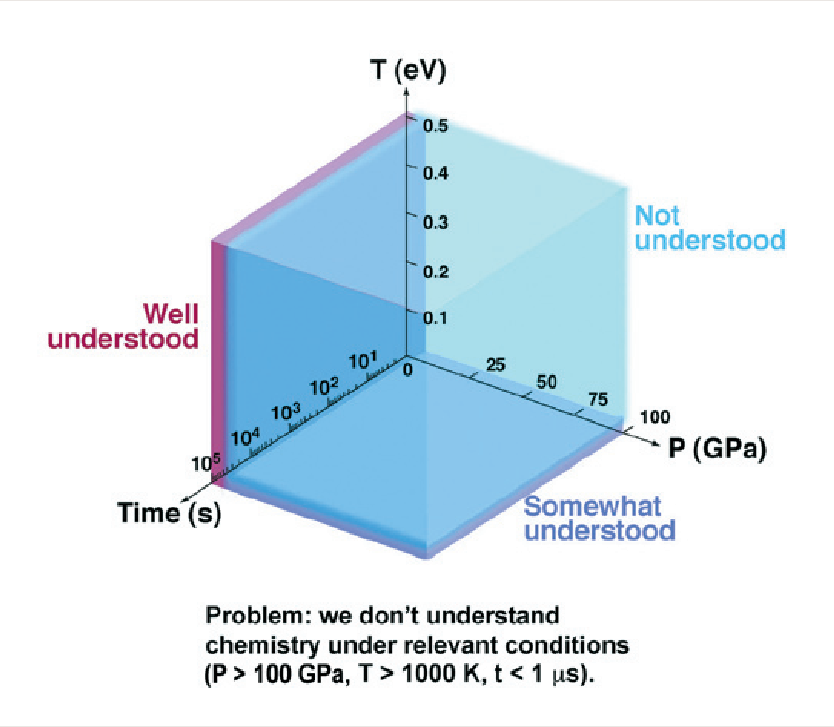
Understanding dynamic chemical processes at high temperatures and very high pressures in the condensed fluid phase is a core need of researchers in several Laboratory programs. This research area is particularly relevant to those concerned with high explosives, verified in situ destruction of chemical or biological weapons of mass destruction, and the possible origins of life on this planet from interstellar delivery of organic molecules.

The fundamental question of how chemistry proceeds at short timescales in pressure-dependent space remains unanswered. Answers to fundamental questions about dynamic chemical processes—such as how and when molecules dissociate in a shock process or what new states may form—also are a first step. We need to understand, for example, how the reaction products of explosives are formed or how simple interstellar organic molecules can polymerize in an impact with a comet. Equilibrium (thermodynamic, chemical, ionization) is often assumed in shock experiments based on the rapid collision rates in condensed systems at high pressures and temperatures, but no one has performed experiments to determine how and when it is achieved. At extreme conditions, the validity of our conventional chemical notions is unclear.

With our extreme chemistry initiative formally heralding a new epoch in chemical research, Livermore has the opportunity to lead the world in fast, time-resolved experimental research and form the tangible basis for guiding the evolution of emergent computational chemistry codes. Chemical synthesis at 10 to 200 gigapascals and 500 to 4000 kelvins is unique, and our initiative will provide a test bed of experiments to validate our theoretical research. National security and the continuing decline of stockpiled weapons systems in favor of smaller and reliable long-lived systems will depend heavily on what we learn about transient-state chemical processes and on the ability to control the synthesis of molecular engineered materials and chemical instruments.

Program Challenges

Large-scale computations of these problems are becoming common. The Laboratory has developed a robust modeling effort through the Advanced Simulation and Computing (ASC Program to model important chemical processes over appropriate timescales and degrees of complexity. Ab initio techniques, although powerful, are limited to the amount of real time they can simulate, typically tens of picoseconds. At longer time frames, chemical models are now required to extend these techniques to predicted chemical processes; however, the models require information about kinetic pathways. Little or no experimental data is available to test



We are seeking to advance our understanding of chemical processes that occur at short timescales under extreme conditions of temperature and pressure. This understanding is relevant to our defense mission and basic research areas, such as planetary science.

and validate ab initio simulations or chemical models. What researchers at the DOE national laboratories do have are measurements of bulk properties such as equations of state, temperature, and electrical conductivity. None of these methods provides direct information at the molecular level. The large temporal gap between simulations (tens of picoseconds) and experiments (nanoseconds and greater) makes comparisons with existing data difficult.

By implementing this strategic objective, CMS will significantly advance the knowledge base needed for high-explosives-driven technologies, including those employed in the nuclear stockpile. Biological studies of systems at high pressures and temperatures can define boundary conditions for motility and reproduction. This information will be valuable to researchers with homeland security objectives. New Laboratory programs will likely be developed in these technologies, including:

Agile design: The ability to design new advanced weapon systems without a long lead time. The basic understanding of high-pressure chemistry will play an essential role as both nuclear and conventional weapons are modernized or redesigned.

Extreme forensics: The ability to characterize explosive events on the basis of their postdetonation by-products. This capability would play a vital role in future national security missions. In addition, truly smart organic, solid-state detection devices will need to be developed for homeland security. These mass-produced, border sentry-agent detection systems (a new paradigm in molecular systems design) will require intense study at the interface between organic chemistry and solid-state chemical systems.

Agent defeat: The use of chemical energy, the most viable means known, to destroy chemical or biological agents during conflicts. The reliable defeat of these agents with chemical energy is one of the most challenging defense problems of our time. Agent defeat combines the problems of explosives technology with those of high-temperature combustion. The extreme chemistry initiative will allow, for the first time, the start-to-finish engineering and modeling of best-case, agent-defeat scenarios.

S&T Challenges

The lack of knowledge about chemical reaction pathways and rates under extreme conditions and the end states of chemical processes hinders the reliable design of systems based on traditional high explosives, new nano-based composites, and organics. Many fundamental questions are unanswered in chemistry, condensed matter physics, and planetary sciences. We expect three key technologies to help us address these challenges during the next six years:

COMET, a laser-driven shock system with picosecond laser diagnostics: Shock experiments based on powerful laser sources such as COMET offer advantages in cost, repetition rate, and flexibility over traditional gas guns.

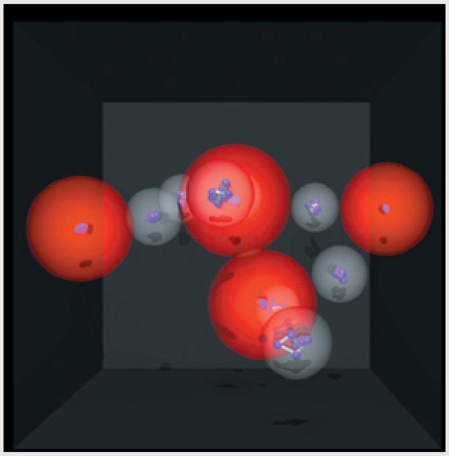
FastDAC, a laser-heated diamond anvil cell system with ultrafast (femtosecond and picosecond) laser diagnostics: FastDAC combines, for the first time, traditional diamond anvil cells with laser-heating and ultrafast laser diagnostics.

First-principles modeling of chemical reactions on long timescales: Layered simulations will combine atomistic models with the high-pressure chemical kinetics of the CHEETAH code.

Our shock experiments, diamond anvil cell experiments, and simulations operating for the first time in overlapping regions of pressure, temperature, and time will validate current simulations of chemical reactions under extreme conditions provided by ASC computers. Simulations will also focus on the calculation of spectroscopic observables, a problem rarely addressed in first-principles simulations.

In addition, CMS will be able to complement the flexibility of shock simulations with the accuracy and thermodynamic controls afforded by diamond anvil cell experiments. Experiments will be performed on simple molecules. Our initial focus will be on identifying one or two key chemical reaction pathways and providing quantification for the first time.

The directorate expects that by 2014, the three key technologies will have developed into stable and robust tools for studying a wide range of problems. CMS will have progressed from understanding a handful of simple chemical reactions to developing networks of chemical reactions, much as is done in gas-phase combustion studies today. As reaction networks grow, CMS's predictive capabilities in high-pressure chemistry will increase, allowing us to predict for the first time how new materials will behave under extreme conditions. A possible scientific breakthrough may well be the first unified and predictive models of giant planetary interiors and atmospheres.



First-principles modeling includes atomistic simulations of nuclear quantum effects.

Advanced Materials Synthesis and Chemical Engineering

Strategic Objective

Our goal is to drive revolutionary advances in the design of new materials while providing effective leadership to meet the changing materials needs of Laboratory programs, particularly in the areas of high-energy-density and energetic materials.

The success of many Laboratory programs is directly tied to the synthesis of new materials. Programmatic needs range from nanocellular foams for targets for NIF, to new catalysts for fuel cells, to designer materials for next-generation sensors. In meeting the programmatic challenges, members of the CMS Advanced Materials Synthesis group have developed a broad range of capabilities in synthetics, including organic and inorganic synthesis, polymer design, and sol-gel chemistry (for which CMS is recognized as the world leader).

Program Challenges

CMS, particularly its Advanced Materials Synthesis group, plays an important role supporting science-based stockpile stewardship, a core national mission of the Laboratory. One active area of involvement is materials design for high-energy-density-science (HEDS) experiments. The complex nature of the materials and structures associated with HEDS experiments—including high- and low-*Z* aerogels, full-density plastics, and low-density metal foams—presents significant challenges in the realm of advanced materials synthesis. As specifications of HEDS experiments evolve, CMS will need to develop reliable synthetic methods that allow for the creation of density gradients, incorporation of dopants, and control over mechanical strength in these materials. CMS expertise in sol-gel and polymer science has enabled the directorate to meet the current demands of HEDS experiments. To stay scientifically ahead of the programs, however, CMS must address many fundamental science issues associated with materials synthesis. These issues are outlined in the next section. The Laboratory's focus on HEDS provides the AMS group with the opportunity to further its leadership in the design of advanced materials that not only support HEDS but also leverage other Laboratory investments, such as fuel cells, waste remediation, and sensor design. Two areas of particular interest follow.

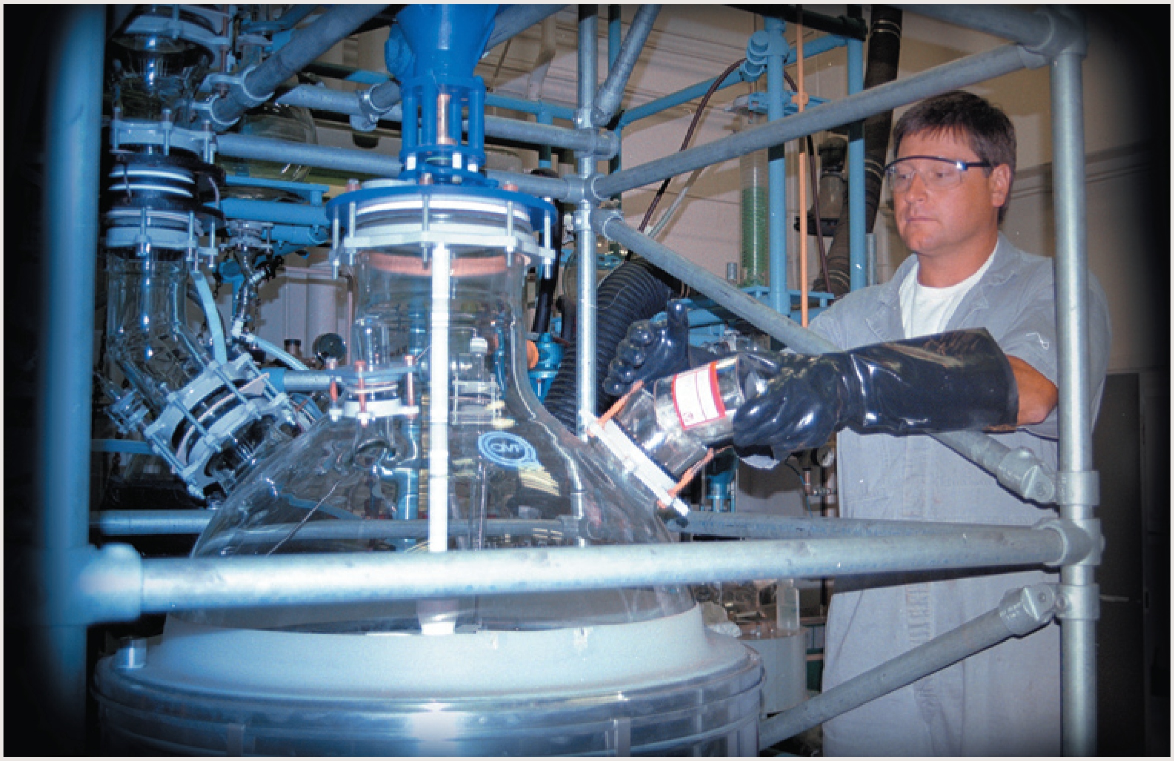
Energetic materials: The synthesis of new high explosives and energetic nanocomposites represents another key scientific and programmatic activity for the AMS group. Much of the energetic materials research at Livermore is focused on the discovery and development of new, more powerful high explosives that are remarkably insensitive to high temperatures, shock, and impact. The use of insensitive high explosives (IHEs) significantly improves the safety of modern nuclear warheads and increases the safety and survivability of conventional munitions as well.

Sol-gel chemistry has been the key to development of energetic materials with improved or entirely new properties. Above, chemist makes a sol-gel to create an energetic material (background).

This effort also addresses the needs of both Department of Defense (DoD) and DOE weapon designers for safer and smaller weapons with increased performance. Continuing and new research efforts seek to find IHEs with significantly greater explosive power than TATB (triamino-trinitrobenzene), the benchmark IHE because its resistance to heat and physical shock is greater than that of any other known material of comparable energy. (Additional information on advances in IHEs is available on the Web at www-cms.llnl.gov/s-t/llm.html.)

For energetic nanocomposites, we seek to develop and characterize novel materials in an effort to maximize storage density of chemical energy while meeting the precise vulnerability, cost, and safety goals of both advanced and conceptual ordnance systems. As the U.S. Army Command meets demands for a greater standoff distance from the enemy, the development of new gun propellants to increase the range of the gun becomes increasingly important. Recently, some high-nitrogen compounds were found to have effective burn-rate modifiers, and serendipitously, they also increased the barrel life of the guns. In a joint effort between modelers and synthetic chemists, models will be derived to allow better understanding of the factors that affect the burn rate of gun propellants and help guide the materials chemist in the development of new, high-nitrogen burn-rate modifiers.

NIF optics: Supporting development of optical materials for NIF is another focal point. NIF is the largest laser and the largest optical instrument ever built, requiring 7,500 large optics (each more than 1 foot across) and more than 30,000 small optics. The success of the pioneering NIF program relies on CMS researchers to sustain and enhance research in the disciplines of chemistry and chemical engineering of optical materials. The design, manufacture, and assembly of these sophisticated components call for innovative ways to make optics of higher quality than ever before and to do so at unprecedented scale and speeds.



After synthesis in a lab, a new explosive is scaled up in a pilot plant at Site 300.

S&T Challenges

One of the most significant scientific challenges facing CMS concerns materials synthesis and involves shifting focus from synthesis of structure to synthesis of function. The ability to design and synthesize, in a rational manner, materials with defined chemical, biological, and physical properties is the central mission of the directorate's AMS group. The materials can range from discrete molecules such as biological receptors or quantum dots, to monolayers for tunable surfaces, and to extended structures such as sol-gel polymers or metal foams. To optimize the level of control in producing custom-designed materials, CMS must develop a fundamental understanding of the mechanisms associated with the synthesis of these materials and gain insight into the structure–property relationships of the final products. These issues will guide "discovery science" and create new scientific opportunities within LLNL and with the outside scientific community.

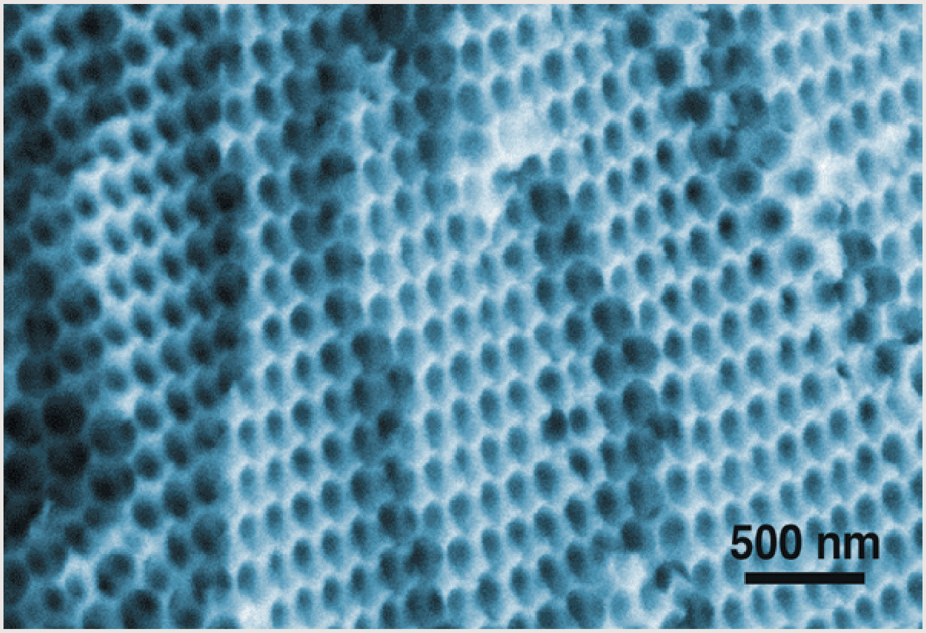
Synthesis research will also provide a new challenge for multiscale materials modeling and simulation: For example, sol-gel-derived organic and inorganic foams represent critical components in HED target design. One shortcoming of current sol-gel chemistry, however, is the inability to reliably control and predict the bulk physical properties of these materials. Control over these properties requires a fundamental understanding of the mechanisms by which solution species form, aggregate, and assemble into the gel network and how these processes influence the physical properties (e.g., cell size, density, mechanical strength) of the resulting sol-gel materials. This understanding, which has not yet been realized for sol-gel materials, will revolutionize the way these materials are made. In addition, the effect of this discovery science will extend beyond HEDS into applications such as sensor design, catalysis, separations, and ceramics.

In the area of energetic materials, the AMS group probes the basic mechanisms and characteristics of energy release. Materials studied differ dramatically from conventional energetic composites; many are heretofore unknown. Understanding basic mechanisms at work in these materials allows for optimizing the performance in these energetic nanocomposites. (An article explaining how nanoscale chemistry can help yield better explosives can be found on the Web at www-cms.llnl.gov/s-t/nanoscale_chemistry.html.)

Currently, the benchmark high explosive for fragment energy is CL-20, a caged nitramine explosive. Because of continuing efforts to miniaturize new weapon systems, new explosives with greater fragment energies than CL-20 are needed. Toward that goal, we will investigate HED organic compounds composed of new bonding patterns of mainly nitrogen and oxygen.

NIF optics: CMS must lead the innovation and development of new laser optical materials and processing technologies to support the design, construction, and operation of NIF.

As NIF ramps up to full operation in 2008, CMS will play a lead role in challenging research issues for NIF optical materials, including: (1) understanding the effects of impurities on crystal growth; (2) conducting deterministic modeling of the crystallization process for potassium dihydrogen phosphate (KDP), NIF's key nonlinear optical material, and its deuterated form (DKDP) for



The ordered microporous carbon aerogel was prepared using an array of nanopolystyrene spheres as a template. Metal-loaded carbon aerogels represent a new nanomaterial with numerous applications.

developing advanced rapid-growth technologies; (3) controlling and minimizing growth defects and inhomogeneities to optimize crystal performance and alleviate bulk damage; and (4) characterizing the mechanism of surface damage and etch pit growth with sol-gel coatings to design effective mitigation schemes.

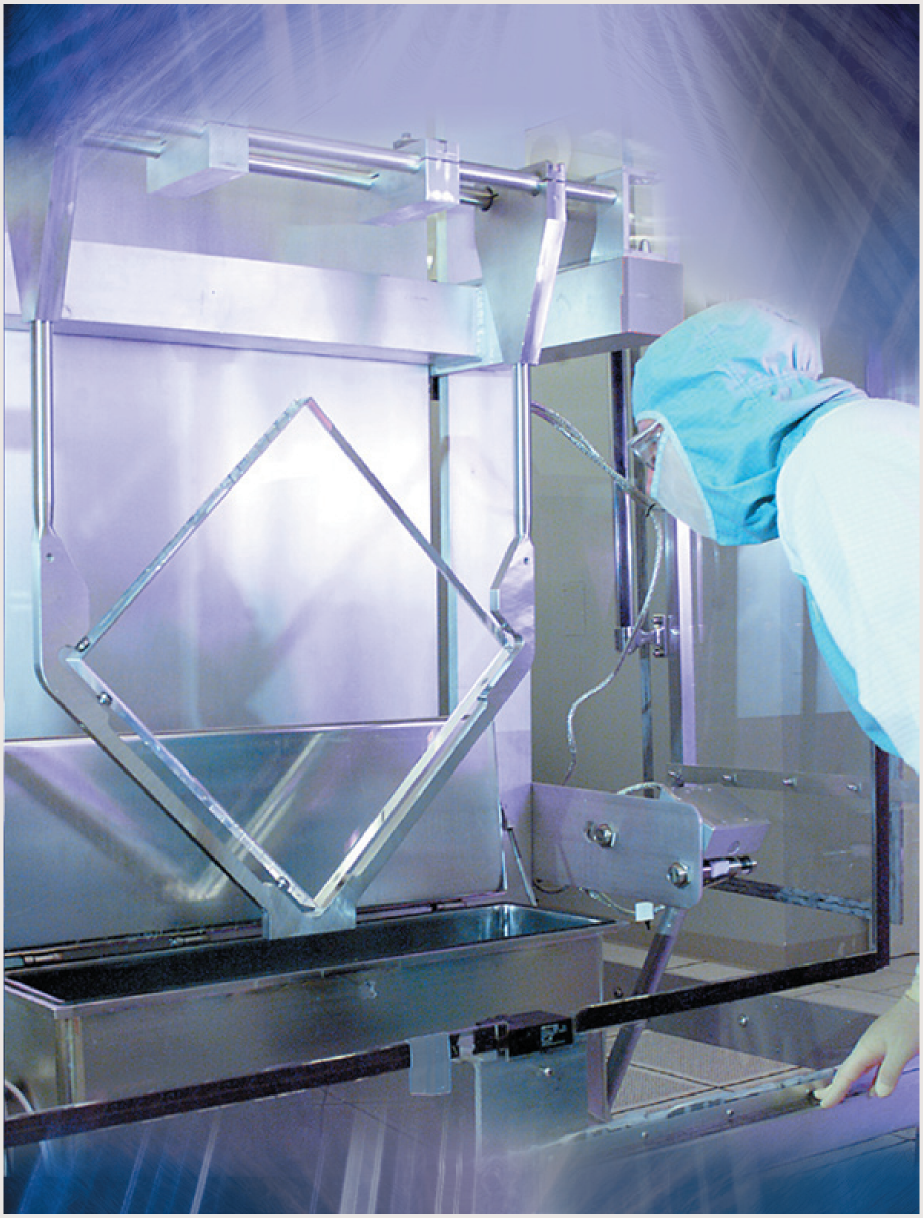
Crosscutting Issues

Strategic themes that are inherently crosscutting include computational chemistry for biology and environment, NIF target synthesis, and weapons materials studies.

Computational chemistry for biology and environment: Researchers in computational chemistry of energetic materials also investigate detonation and slow combustion of explosives, kinetics of high-energy-density materials, and electronic structure modeling for high explosives. This computational expertise has fostered several crosscutting efforts. For example, our scientists are initiating new research on pathomics (the change in protein levels in a body when it is exposed to a pathogen), gene expression and synthesis, and bioaerosol modeling.

In the environmental sciences, we have a strong focus on combustion chemistry simulations of ignition, flame propagation and quenching, and emissions from internal combustion engines. Reaction mechanisms have been developed to study the influence of fuel molecular structure on ignition properties, such as octane and cetane ratings of automotive fuels. We also focus on modeling reactivity and bonding at the water–aerosol surface interface of global climate research. In addition, we are developing kinetic models for surrogate and actual chemical warfare (CW) agents for use in a variety of atmospheric dispersion and other accident and terrorist scenarios. We will leverage molecular modeling and simulations efforts by enhancing these new S&T areas and collaborating with other organizations.

(An article on the role of computational chemistry in the investigation of energetic materials can be found on the Web at www-cms.llnl.gov/s-t-disc/chemistry.html.)



An Optics Assembly Building technician prepares and inspects a slice of KDP crystal, a key nonlinear optical material for the National Ignition Facility.

NIF target synthesis: The synthesis of targets for NIF, one of the most widely crosscutting challenges in our S&T plan, involves aspects of design, prototyping, assembly, and characterization to produce submillimeter-scale spherical targets of significant complexity. This effort requires expertise across the CMS divisions and partnerships with other directorates (NIF, Engineering, and Physics and Advanced Technologies [PAT]). CMS scientists have expertise in polymer chemical processing and coatings, essential for designing NIF targets now and required for future laser development.

Weapons materials studies: CMS weapons materials R&D, associated with science-based stockpile stewardship, cuts across all CMS divisions and relies on strong partnering with the DNT and PAT directorates. Programmatic challenges lie in how CMS technical representatives are embedded in DNT's A, B, and W Programs. Scientifically, we must revitalize R&D efforts in several areas, including metals, polymers and organics, aging and compatibility, surface science, and component- and system-level modeling. For example, strengthened experimental efforts are needed in uranium chemistry, particularly regarding corrosion and aging. We also must develop better assessment tools for organics aging, compatibility, and replacement issues. Efforts to renew two- and three-dimensional system-level modeling (e.g., mechanisms and kinetics) are also needed. An additional strategic need is the preservation of a weapons materials knowledge base, possibly expanded through development of a Web-accessible database.

Workforce Requirements

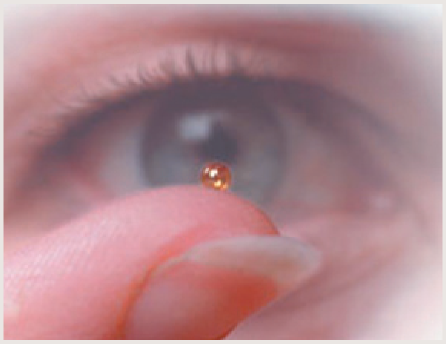
To maintain leadership and broaden the scope of CMS scientific capabilities in the areas of extreme chemistry and advanced materials synthesis, CMS must broaden the directorate's personnel base. CMS currently has a strong core of theoretical chemists, synthetic chemists, and experimentalists. However, as DOE programmatic needs evolve and people retire, an enhanced workforce skilled in theoretical, synthetic, and experimental chemistry will be required to meet sponsors' needs and afford new opportunities for discovery science. Thus, our goal is to retain and recruit the most talented workforce for this strategic theme area across all levels, from technical support to scientific leaders.

As the workforce evolves and grows, communication and coordination with other Laboratory programs must be improved. Real improvement will require more than just furthering understanding of customers' needs and missions. The programs themselves need a working knowledge of CMS extreme chemistry and materials synthesis capabilities. The directorate is currently developing this mutual understanding with DNT, and that interaction is driving a number of new scientific activities. CMS capabilities, however, can also leverage a number of other programmatic efforts, and as a result, an aggressive plan is needed to develop these new relationships.

To meet recruitment and staff retention goals in a robust fashion over the long term, we must establish a pipeline of talent. The general approach is to establish interactions at the undergraduate level through summer education programs. Exceptional undergraduate candidates are then brought further into the Laboratory workforce either as B.S.-level hires or as graduate student researchers. For candidates pursuing graduate school, our logical next step is to hire them as postdocs.

In parallel, we will recruit talented graduates or early-career staff by enhancing our visibility in the national science arena through participation in meetings, workshops, and seminars. We envision that in the next five years, we will need to recruit exceptionally gifted mid- or late-career leaders in both the extreme chemistry and materials synthesis areas to aggressively lead our younger staff into the future.

Strong collaboration and communication will be the central themes for implementing and fulfilling a workforce plan for strategic objectives. For extreme chemistry, external relationships include continuing the established collaborations with the University of Utah and interactions with California Institute of Technology through the ASC University Centers. CMS also is exploring a range of possible



The technology to make hollow laser-target shells for NIF is being refined.

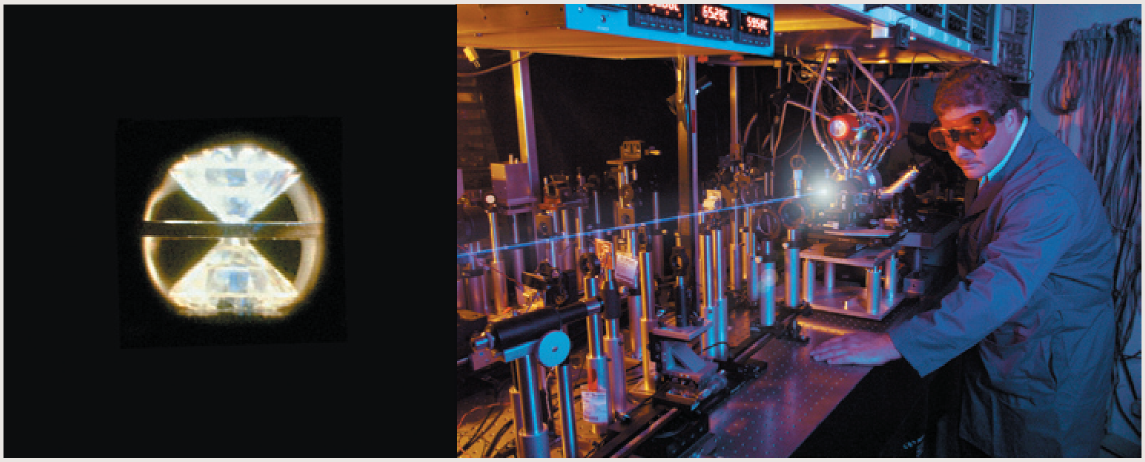
extreme chemistry interactions with personnel on UC campuses (e.g., UC Riverside, UC Irvine, and UC Berkeley). For example, one possible collaborator from UC Berkeley is a world-renowned expert in planetary chemistry as well as a former chair of the JASONS review board. That involvement will help to strengthen ties between the Laboratory, UC Berkeley, and Lawrence Berkeley National Laboratory in this area. This collaborative effort will help efforts of the high-pressure consortium at the Advanced Light Source at LBNL.

CMS is responsible for the maintenance and stewardship of our chemical engineering workforce, which is heavily matrixed across DNT, NIF, and NAI. Future principal needs are projected to be in chemical processing for energetic materials, process engineering for NIF optics, and chemical and nuclear plant engineering expertise for NAI. Successful support for these programs as they address scientific and technical challenges requires implementing a more generic recruitment strategy geared more toward university and industrial partnering rather than the purely academic collaborative approach. (See the Web version of the strategic plan for additional workforce considerations.)

Infrastructure Requirements

CMS proposes to develop at the Laboratory an extreme chemistry center for use by multidisciplinary teams to solve challenging scientific issues that extreme chemistry presents. The center's primary components will be a fast diamond anvil cell (FastDAC) laboratory, which will combine laser-heating DAC technology with fast laser spectroscopy diagnostics to initiate and monitor chemical processes at extreme pressures and temperatures, and a tabletop shock laboratory, which will provide CMS with a resource for high-speed, laser-driven shock experiments.

A materials characterization facility dedicated to analysis of advanced materials is also needed to improve our understanding of reaction mechanisms and structure–property relationships, which are of paramount importance in the design of new materials. The facility should contain equipment for thorough compositional and structural characterization and for assessments of bulk physical properties such as mechanical strength, conductivity, and magnetism.



Light-induced ultrasonic studies for new and aged explosives are conducted at high pressure and temperature using heated diamond anvil cells (left).

Science at the Intersection of Chemistry, Materials Science, and Biology

This research theme focuses on the fundamental investigations of the properties and performance of materials at the intersection of chemistry, biology, and materials science for developing a new generation of chemical and biological sensors.

Vision

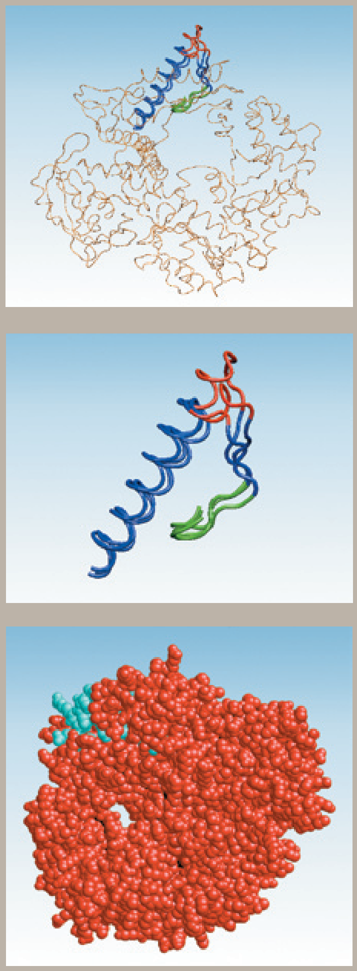
To provide the fundamental scientific capability to synthesize complex molecules and measure and track molecular interactions in complex environments in support of Livermore's mission in sensing and to sustain a strong life-sciences effort at Livermore. To fulfill this vision, CMS will forge strong external alliances, expand its hiring efforts in this area, partner more effectively with sponsors, and continue to invest in signature analytical capabilities.

Strategies for Change

The science of the new century will continue to emerge at the boundaries between historically separate disciplines. Over the last few decades, rapid progress in what is being termed chemical biology has already enabled the laboratory synthesis of a whole virus and detection and analysis on the single-molecule level. Extraordinary breakthroughs in nanoscience give us the ability to interface individual molecules with macroscopic devices. Engineering this inorganic–biological interface simultaneously creates thrilling science and initiates many challenges for CMS.

This science is also mission-critical for the Laboratory. Two years after 9/11, defense organizations were still playing out scenarios with six-figure fatalities from small terrorist groups. The Laboratory and CMS have the opportunity—and the duty—to help prevent such scenarios from becoming reality. While our historical national security mission remains central to the future of CMS in other strategic areas, developing sensors to counter weapons of mass destruction (WMD) is our top priority in driving science and technology for chemistry, biology, and materials science. We believe that the best countermeasure to a $400 kilogram of botulinum is a sub-$10 sensor. Nanotechnology plays a key role in making detection systems massively parallel and cheap. Biomolecular interfacing and sensing will also lead to breakthroughs in other mission-critical applications. Applications from molecular recognition to environmental remediation and human health are obvious. The analytical and sensor-integration efforts discussed here also support our missions in defense and stockpile stewardship.

Multidisciplinary missions put the Laboratory in the middle of exciting scientific problems and require us to actively collaborate with the broader community. Missions in nonproliferation and counterterrorism can only be accomplished by the national labs if they work in strong partnerships with both academia



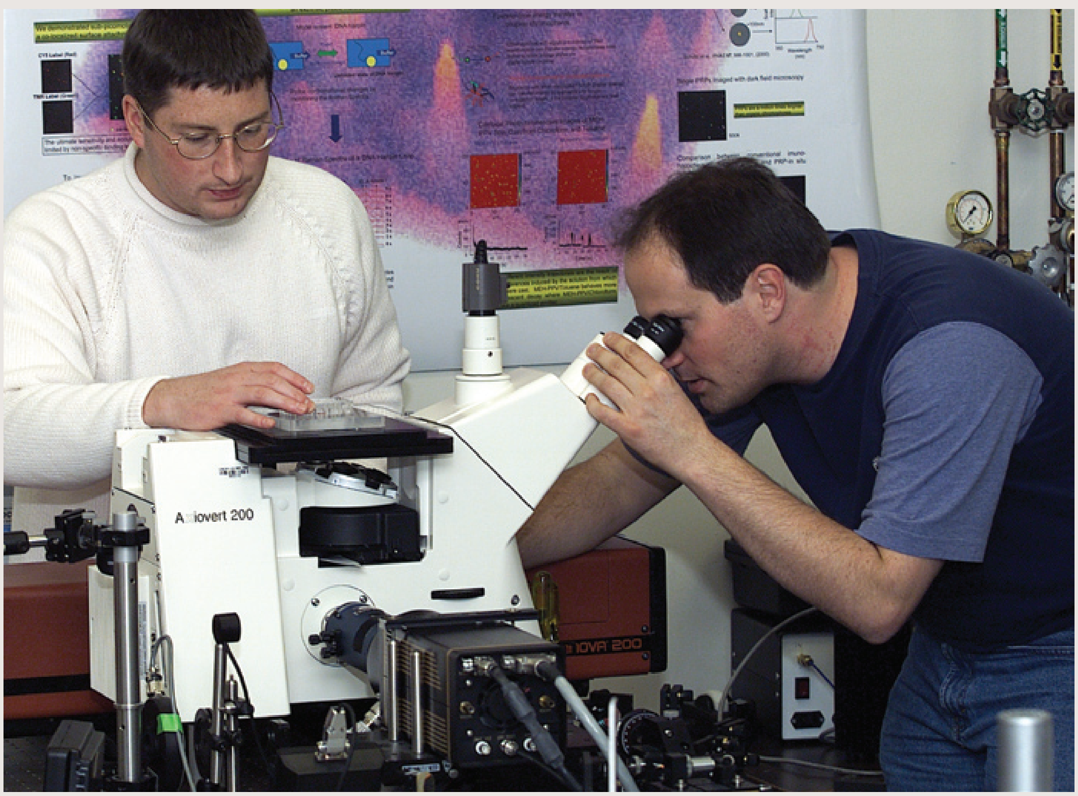
In this model of a pathogen protein, blue represents the part that is conserved in all strains of the pathogen's DNA, red represents the portion that is unique to the target strain, and green depicts the most highly conserved portion across multiple organisms. The DNA-based signature combines those portions of DNA that code for both the blue and red regions.

and industry. Livermore has played a leading role in defining homeland security science and technology since before the creation of the federal Department of Homeland Security (DHS). This role will likely continue in the future, but the science to support homeland security cannot be conducted exclusively at a national lab. The required effort will drive Livermore and CMS to develop much closer connections to the broader scientific community, academia, and industry. We expect academia to have a dominant role in the underlying science, and we expect industry to have the lead in deployments and in cost-reduction. Livermore occupies key middle ground by integrating new ideas and building the first prototypes.

We will also need to partner much more effectively with a broad range of sponsors. Funding for homeland security is complicated. For example, the National Institute of Allergy and Infectious Diseases, a part of the National Institutes of Health (NIH), has emerged as a national security sponsor, but it remains invisible as a program within the Laboratory. The DHS Homeland Security Advanced Research Projects Agency controls the pathway from prototype to deployment, and Livermore must develop a coherent approach to interacting with this agency. Because the technologies for homeland security have multiple uses, opportunities abound for leveraging DHS-driven science and technology to obtain funding from institutes in NIH as well as from DOE's Office of Biological and Environmental Research.

Although the homeland security mission gives Livermore enormous opportunities, it also presents immense technical, cultural, and structural challenges. This section lays out CMS's plan for meeting these challenges in three critical areas that drive chemical sensing (including radiological chemistry) and biosensing. These areas are:

- Molecular recognition.
- Analytical sciences.
- Systems integration.



Chemists use a wide-field-of-view fluorescent microscope to image single molecules.

Molecular Recognition

Strategic Objective

Our goal is to lead the world in understanding molecular recognition systems and in demonstrating novel systems with extraordinary affinities and exceptional stabilities for measuring and tracking complex molecular systems.

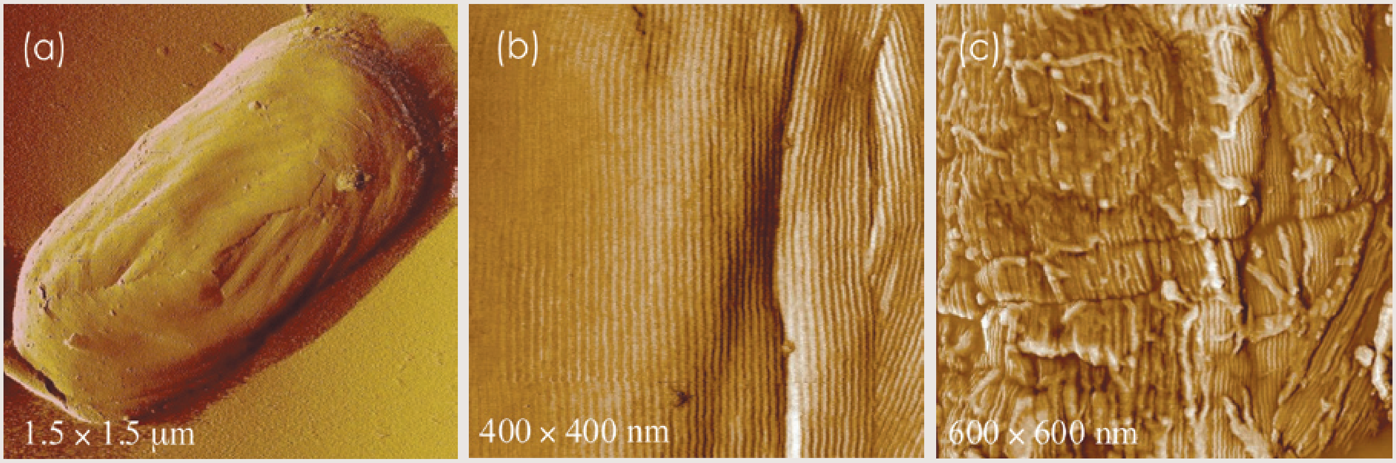
The heart of any chemical or biological sensor is the molecular binding event. The transducer in a sensor responds to a given concentration of the bound analyte. Biological molecular recognition systems typically have affinities in the micromole to nanomole range, but the sensitivity required for biosensors in many applications for DHS is in the picomole or even femtomole regime. The performance of a sensor is more often dominated by the specificity, which is the ratio of the binding of the target analyte to the binding of all background molecules. Unfortunately, we have as yet no means to quantify the chemical and biological backgrounds.

Program Challenges

The most fundamental issue in countering WMD is the breadth of possible targets. This means that we must sense all possible chemical, biological, and radiological threats. The threats include chemical warfare agents as well as every imaginable chemical, all human-pathogenic viruses, bacteria and their associated toxins, agricultural pathogens and engineered agents, and all radioactive isotopes. Currently, toxic-chemical sensors and immunoassays exist for many compounds, a few toxins, and about 20 pathogens. The key to homeland security is developing sensors that span the entire range of possibilities. Radiation detectors for homeland security must similarly detect a far wider range of materials and energies than an application-specific detector.

False positives remain a problem area for most low-cost chemical and biological sensors. Most deployed radiation detection systems also have sensitivities limited by the tolerable rate of false positives. However, in an emergency or response scenario, time is the most important component.

The need is critical for advancing the scientific understanding of backgrounds and quantifying false positives. Radiation backgrounds may be orders of magnitude higher than the signal to be detected. Biological backgrounds may be six orders of magnitude higher than the signal to be detected. The lack of substantial information on backgrounds undermines the ability to establish meaningful performance metrics for molecular recognition efforts.



These images resolve the shape and surface features of a Bacillus subtilus niger *spore (surrogate for anthrax). A hydrated spore (a) is magnified in (b), showing a surface consisting of arrays of rodlike structures that fold when dehydrated (c).*

S&T Challenges

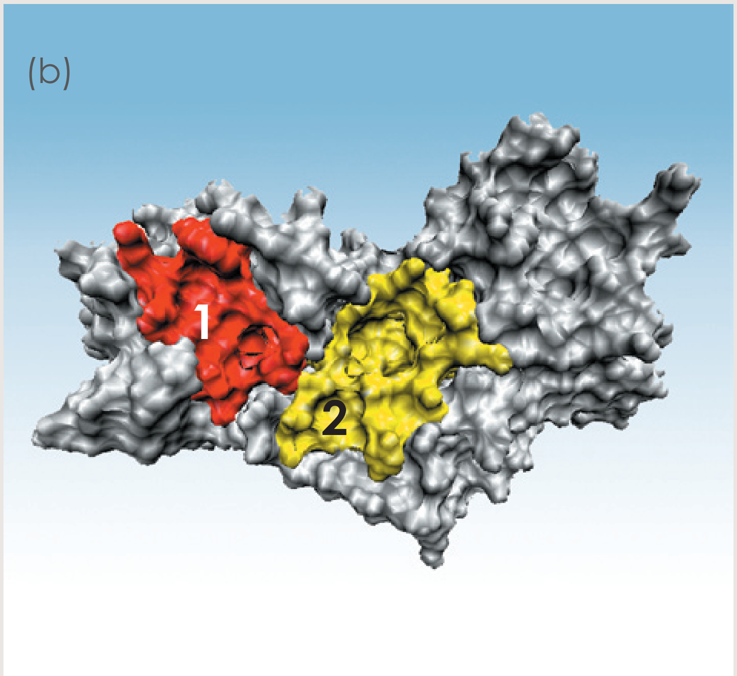
The central challenge in molecular recognition synthesis is designing materials and chemicals that display specific interactions with known targets. Understanding molecular recognition in vivo is at the heart of DOE's Genomics:GTL (formerly Genomics to Life) Program. Accomplishing this requires both better synthetic and computational tools than we currently have.

We continue to expand our capabilities in chemical synthesis by incorporating novel techniques. Synthetic routes have been established to create DNAs, proteins, and a complete virus. CMS effort is focused on molecular recognition of WMD, but other LLNL applications could include environmental remediation, catalytic synthesis, and energy generation and storage.

The logical extension of biochemical approaches to synthesis is the use of genetically engineered living cells as chemical reactors. This approach is becoming widespread. Its importance in the molecular-recognition arena is that it can use many cellular biochemical routes to perform molecular-recognition tasks of interest to homeland security.

The interaction of complex chemical and biochemical molecules controls the processes of life but it is only qualitatively understood. The Laboratory's Blue Gene/L supercomputer should enable the quantitative computational study of these interactions and transform our understanding of biochemical processes. However, effective use of this tool calls for improved computational techniques and algorithms.

The field of radiation damage in living organisms has yet to feel the effect of synthetic and computational tools. However, these tools should eventually make possible detecting radiation dose to extremities (fingers) and to microbes. The ability to use protein signatures to diagnose exposure could advance the understanding of how to mitigate or provide resistance to radiation exposure. Developing this capability should be a priority.



(a) The x-ray crystal structure for the tetanus toxin shows how the amino acid chain is folded and (b) its calculated molecular surface shows the predicted binding sites for ligands (sites 1 and 2).

Analytical Sciences

Strategic Objective

We want to build on the Laboratory's heritage in analytical sciences to enable quantitative measurements of chemical and biochemical systems and to develop techniques and prototype tools that will provide a real-time capability to quantitatively analyze complex systems.

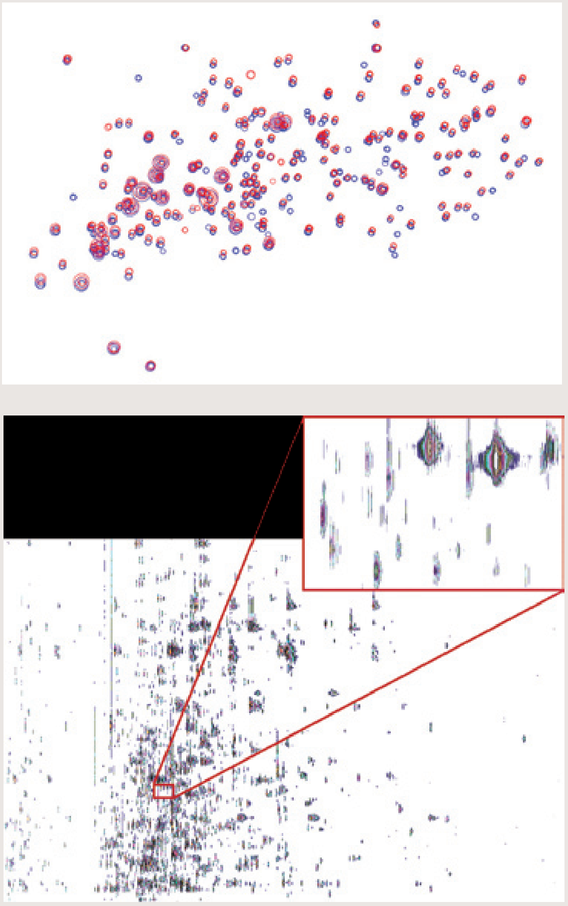
Analytical tools support sensing in the broadest sense. Advanced laboratory techniques extend the boundaries of what is measurable. The current tool set borrows heavily from Livermore's long-term investments in analytical tools that support the stockpile stewardship and nonproliferation missions. Ultimately, analytical science forms the foundation of our mission in sensing because every fielded sensor and analytical approach is demonstrated first in the lab. Moreover, laboratory-based analysis forms the core of sensing for attribution. Our ability to push the limits of what is measurable is our competitive edge.

Program Challenges

Analytical challenges call for extreme flexibility in instrumentation and workforce. Because targets for lab analysis are almost infinitely varied and the sample matrix is generally far more complicated, development of real-time analytical and separation techniques and protocols is of intense interest. For example, clues to a sample's origin may come from growth media, compositions, impurities, isotopic geolocation, and precision isotope dating of samples. We will continue to transfer techniques to our partners at standard analytical labs such as the FBI's.

The Forensic Science Center (FSC) has the ability to handle "all threat" unknown samples and internationally recognized expertise in WMD forensic analysis. (See sidebar on pp. 35–36.) However, maintaining this expertise is difficult without investing in new instrumentation. It is critical that we fund instrumentation and science and technology to steadily upgrade FSC's capabilities.

Remote sensing remains a crucial national security activity that CMS supports. Remotely controlled active (laser) sensing and passive sensing are possible, but they must meet stiff requirements. Chemical and biological weapons possess characteristic infrared spectral features throughout the so-called fingerprint (3- to 12-micrometer) region. Key challenges are in the mid-infrared (3- to 5-micrometer) region and the long-wave infrared (8- to 12-micrometer) region, which require tunable output lasers or high-resolution spectrometers.



We are developing techniques to analyze the proteins in blood serum and quickly detect the presence of a pathogen long before someone becomes sick. The researchers use liquid chromatography to separate and ionize chunks of serum protein before they are analyzed by a mass spectrometer (below). Above is a snapshot of serum proteins. When the two colors are separate, it indicates a protein is changing.

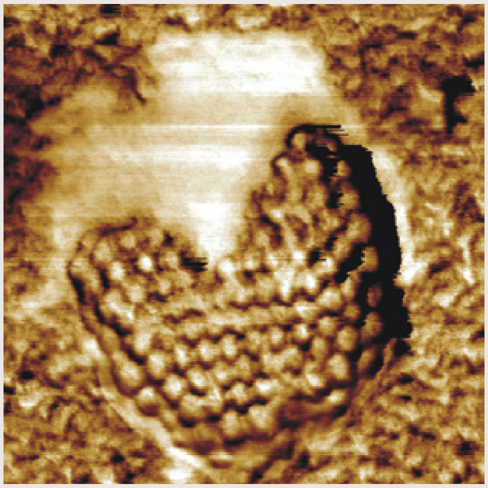
S&T Challenges

The emerging science of bioimaging has broad applications for CMS and deserves greater attention than it has received in the past. Bioimaging provides information on the pharmacokinetics of toxins as well as medicines and gives a detailed view of how isotopically marked species propagate through a cell, both of which are central to Livermore's role in DOE's Genomics:GTL Program.

The underpinning of bioforensics is a complete understanding of key chemical pathways. Thus, bioforensics is closely tied to our role in Genomics:GTL, the follow-on to the Human Genome Project. The Center for Biophotonics, a major Livermore asset for work on Genomics:GTL, should be more fully leveraged to support other Laboratory efforts. For example, the ability to measure isotopic ratios in minute detail also bears on both bioforensics and planetary-scale atmospheric models. Extraordinary science problems are becoming computationally tractable with the new generation of machines. Understanding the proteomic architecture of pathogens and the dependence of that architecture on species, strain, and processing is key to identifying target molecular signatures for molecular recognition. Molecular signatures also provide a crucial scientific foundation for a bioforensics capability.

The maturation of technologies such as single-molecule optical imaging and spectroscopy, along with force imaging and spectroscopy, opens the door to investigating protein interactions and complex formations. These phenomena underlie binding events at sensors, formation of molecular machines that carry out cellular function, and the propagation of disease. Livermore also has a leadership role in chemical force microscopy, an emerging technique that offers the prospect of complete understanding of the physical forces generated by interacting biological molecules. Regions of special spectroscopic interest are the mid-infrared, terahertz, and microwave. Remotely interrogated, semipassive probes appear to offer the perfect compromise.

A researcher uses atomic force microscopy to learn how the protein osteopontin can control the growth of a kidney stone.



This atomic force microscope image of herpes simplex virus-1 (HSV-1), one of the most widespread human viruses, shows its outer capsomere structure.

The Forensic Science Center

The Forensic Science Center (FSC) provides chemical and forensic analysis capabilities in support of chemical, nuclear, and biological counterterrorism. Recently, the FSC has undergone reorganization and refocusing of its programmatic mission. Concomitantly, the FSC is developing a basic and applied science and technology portfolio that will support the long-range mission of both historical and new partners. The FSC is also creating new relationships within LLNL organizations to better support its programmatic customers.

The FSC has a unique position as one of a limited number of facilities in the nation that can accept, analyze, and attribute all-threat, unknown samples in a wide variety of matrices. We are leveraging that expertise in a number of ways to support our established sponsors and providing scientific, technical, and programmatic planning leadership to emerging national and interagency homeland security efforts. We deliver scientific insight and solutions to real-time national security, nonproliferation, and intelligence situations.

The FSC has been heavily engaged in world and national intelligence interests, and more recently, in domestic security support for federal law enforcement, including the FBI, FDA, and Customs (now a part of DHS). In the past, the FSC's funding level at any given time was quite variable and dependent upon a number of work-for-others projects, but the center is working toward a goal of broad, common, and leveraged investment with sponsors that can benefit from our activities. These refocused activities are also driving the direction of our science portfolio. We are developing four areas of basic and applied science that map to the long-term strategic needs of our sponsors. These four areas are:

- Analytical science and new instrumentation development.
- New materials synthesis for collection, detection, separation, and preconcentration.
- Nuclear science in support of forensic analysis and attribution.
- Bioforensics (chemical signatures of biological processes).

Scientific growth in the FSC is multidisciplinary, so we are teaming with a number of different centers and institutes within LLNL. We are also aggressively teaming with NAI scientists to enhance the science portfolio for all of NAI. By developing a strong multidisciplinary and multiprogrammatic approach—including postdoctoral researchers—to the FSC science portfolio, we hope to strengthen our position for continuing institutional funding for instrumentation reinvestment, as recommended by the last NAIC review committee.

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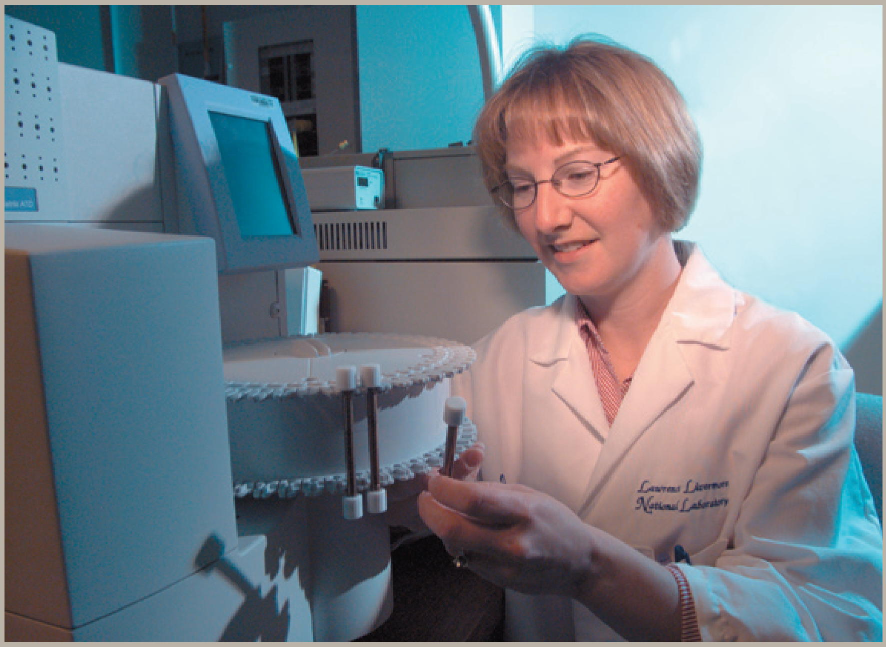


A chemist in the Forensic Science Center readies samples for testing.

The Forensic Science Center (continued)

The FSC is also developing new strategic theme areas that will support current and future NAI programmatic directions. They include:

Forensic analysis of unknown WMD: The FSC is in a unique position nationally to be both a sample receival and analysis center for unknown samples. We are working closely with the LLNL Chemical and Biological Nonproliferation Program (CBNP) for implementation.

Explosives detection and analysis: This includes new real-time detection and field screening for traditional and nontraditional explosives and energetic materials.

Training for first responders, initially targeted toward the National Guard civil support teams (CSTs): In a state or local situation, the CSTs bridge the gap between local and federal response. Fifty-five teams are currently being set up, at least one in each state and four territories, with two in California. Training under development via the FSC focuses on the science of weaponized chemical and biological agents, methods development, and exploitation of current technology available for the teams.

Bioforensics in support of the LLNL CBN program: As the Department of Homeland Security is fully organized, integrating LLNL bioforensic activities with other national assets, such as the National Biodefense and Countermeasures Center (NBACC), will be critically important. The FSC is working closely with LLNL's CBNP to establish a bioforensic labor-atory that supports programmatic goals and links with other pertinent national partners, such as NBACC.

Forensic Science Center scientists take care to ensure that all test results are properly documented.

Strategic Objective

Our goal is to build the systems understanding and materials technologies that will enable radical new systems approaches for massively parallel sensing and surveillance.

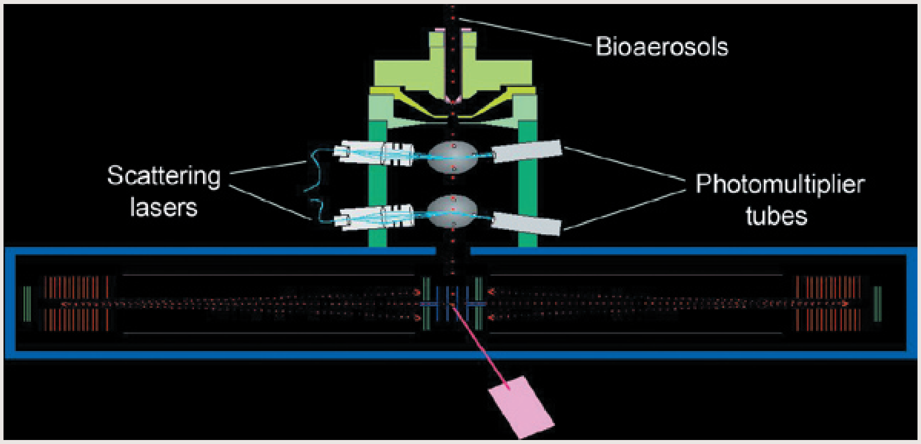
Systems integration has been a key strength at Livermore. DHS will draw on capabilities from across academia for basic ideas, and it will field devices from industrial partners. Integrating scientific concepts into the first working prototypes is Livermore's natural role. More specifically, the CMS role is to integrate materials and develop the fabrication processes to support this systems integration effort. CMS must work with Engineering and with external partners from industry and academia.

Program Challenges

The key challenges involve cost, stability, and operations. We must counteract low-cost threats with even lower-cost countermeasures. To counteract a possible attack using a single container of smallpox, the U.S. is mobilizing both a multi-$100 million vaccination program and a multi-$10 million sensing program. Even at this price tag, coverage using today's sensors is inadequate. A similar issue exists with radiation sensing, where costs limit sensors to those with inadequate resolution to discriminate against background levels. Success in low-cost sensing requires broad external partnerships.

The short shelf life of an activated sensor is a fatal flaw for a low-cost network. CMS must explore potential solutions to the high-false-positive challenge by taking approaches such as chemically "refreshing" the surface on a periodic basis.

The operational challenges are primarily associated with complexity and supply chains. Finding solutions to these challenges should be an important priority.



A schematic of a bioaerosol mass spectrometry system (BAMS) being used to analyze a bacterial spore. BAMS has the potential to identify bioagents, such as anthrax, from only a single spore or cell and to elucidate the molecular changes that occur in normal and abnormal cells.

S&T Challenges

The interface between inorganic and biological materials controls a detector's lifetime, cost, and specificity. Of particular interest are capabilities for interfacing biological and inorganic systems in a controllable fashion; designs such as cantilevers or pores that open up new architectures in transduction; chemistries that detach bound molecules without deactivating the molecular recognition chemistry; and technologies to control and eliminate biofouling. The same capabilities have applications for chemical sensors and medical devices and for the biosciences in general. A strengthened relationship with NIH would greatly enhance Livermore's ability to realize the natural spin-offs in human health.

Science challenges include the controlled and reproducible synthesis of materials that are exquisitely sensitive to their environment. Technology challenges include fabrication techniques that incorporate recognition materials into devices and devices that simplify the transducer in a sensor. New science opportunities are possible from massively parallel, integrated sensing.

Technology challenges include going beyond packed-bead filtration. We will work with the Engineering Directorate to develop separation technologies that use channel geometries that are tightly specified and controlled at length scales close to those of the molecules being separated. Because nonzero flow gradients across biological molecules exert control on molecular geometry, we must develop the ability to design these channels to provide the necessary predictability.

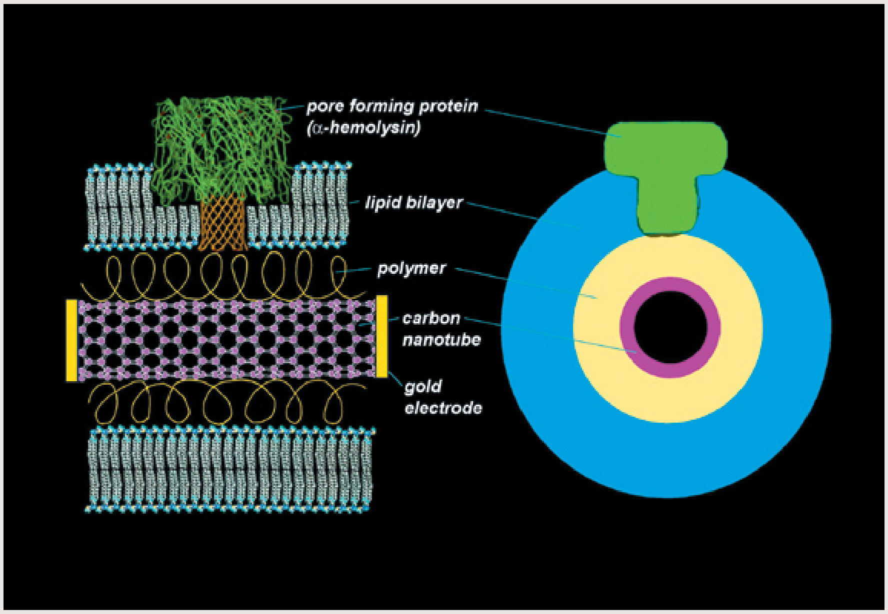
Crosscutting Issues

NIH has emerged as a national security sponsor, but working with the organization remains challenging. It is critical for Livermore and CMS to build a more streamlined method to work with this sponsor.

CMS–NAI program work for DHS will, by its nature, be more closely associated with academia than traditional Livermore programs. In addition, CMS has great opportunities to leverage efforts from outreach and recruiting that are generally the province of the University Relations Program. A number of University of California-based centers offer the possibility of both establishing valuable collaborations in the chemical and biological materials arena and strengthening Livermore–UC connections. In particular, CMS should target the California Nano Systems Institute, the Molecular Foundry, the UC Santa Barbara–Massachusetts Institute of Technology–California Institute of Technology Consortium, and the potential National Science Foundation's Science and Technology Center in Hard–Soft Interfaces at UC Davis.

Program requirements call for a rapid transition in hiring staff with a new skill set, a challenge in a shrinking workforce environment. A single plan for hiring and retraining must be built throughout CMS and coordinated with the other directorates.

The homeland security mission will call for more partnerships with industry. Therefore, strengthening existing partnerships are a crucial part of this plan. The present Industrial Partnerships and Commercialization (IPAC) policies and practices should be modified to help build these relationships. In particular, we must seek a more streamlined process for nondisclosure agreements, a proactive approach to support partnering, and a policy of nonexclusivity in licensing arrangements.



This diagram shows a longitudinal and transverse section of a new type of biosensor that is based on a lipid-coated nanotube. The sensor is designed to detect bacterial toxins that poke holes in cell membranes. The biosensor starts with a rolled-up carbon nanotube that is coated with a layer of polymer molecules and then a bilayer of phospholipids that mimics a cell membrane. With electrodes attached to both ends of the nanotube and a voltage applied, the minuscule sensor can detect pathogen toxins that puncture a hole in a cell—or artificial—membrane.

Workforce Requirements

Correcting the current shortage in synthetic chemists should be the top priority. We should increase the number of synthetic chemists in molecular recognition from 4 to 15 over the next several years. The proposed Institute for Molecular Synthesis will give this group an identity and provide the platform for a senior-level hire. Computational biochemists are our next priority, but this need has received minimal attention so far. The continued blurring of disciplines is likely to increase the need for biochemists and chemists with biological experience or training. Only 1 percent of the CMS population is biochemists; the goal is to increase this figure to about 10 percent over the next decade, as budgets permit.

Spectroscopy has been a traditional strength at Livermore, but CMS does not have a core staff focused on this strategic area. Such a core group should be established.

Biomedical engineers' skills are highly synergistic with CMS strategic goals. These engineers are currently available, in contrast to three years ago. We anticipate hiring two to three junior researchers. Hires of more senior researchers with a strong NIH track record should be pursued. We also have a need, although limited, for device integration and processing engineers to enhance the partnership with Engineering.

Infrastructure and Computational Requirements

Centers and institutes: The BioSecurity and Nanosciences Laboratory (BSNL) and the Forensic Science Center have a range of capabilities that affect development of molecular recognition chemistry. (See sidebar on pp. 41–42 for more information on the BSNL.) Many synthetic chemists within CMS reside in these two centers, and arguably, all current efforts in molecular recognition chemistry are being pursued within them. Moreover, many tools (mass spectrometry, liquid chromatography, and nuclear magnetic resonance) that are needed to analyze synthesis products are located within these centers. Because of the potential benefit of improved coordination between P- and Q-cleared analytical and synthetic activities, we will study the potential of using joint facilities.

The bionuclear initiative of the Glenn T. Seaborg Institute (described in the sidebar on p. 44) helps to link science at the intersection of chemistry, biology, and materials with applied nuclear science, a mainstay of Livermore programs. The institute couples chemical and molecular recognition in molecular-targeted radioisotope therapy for treating cancer. This program is a valuable tool for recruiting both nuclear and chemical scientists; presenting opportunities for high-profile science in radiation detection, radiochemistry, and mass spectrometry; and broadening the CMS sponsor base in health.

Livermore's Radiation Detection Center has a strong national presence in detection systems but with minimal focus on materials. The center should build on its capability to develop room-temperature detection materials.

The proposed Institute for Molecular Synthesis would provide an important capability because it supports molecular recognition as well as integration and analysis.

The proposed Aerosol Test Center would be a key facility for testing integrated devices in a realistic environment. It would be an important element in building the science base of a quantitative understanding of backgrounds, the evolution of bioaerosol properties, and fate and transport.

The BPAC and BSNL requirements: Historically, Livermore has been strong in analytical sciences. The CMS assembly of inorganic-materials analytical tools is loosely referred to as the biophysical analysis capability (BPAC), whose tools include nuclear mass spectrometry, mass spectrometry, scanned probe imaging, and optical spectroscopy. BPAC tools perform analytical work as well as beam analyses in the FSC, Seaborg Institute, and BSNL. Total value of the BPAC suite of instruments is now about $40 million. With an assumed useful lifespan of 10 years, CMS has insufficient funding from the institutional general plant equipment (IGPE) to maintain BPAC's capability at this magnitude; therefore, strong programmatic and institutional involvement in equipment purchases is essential. In addition, because assets are not always well used, a task force should be formed to inventory and survey major capital analytical tools and document any gaps and underutilization.

Mass spectrometry remains the highest-cost and highest-impact technique in the BPAC. We need a plan for IGPE investments in this technology. Centers such as the FSC need a sustainable plan for equipment replacement, especially in mass spectrometry. To attract institutional investment, the FSC must develop a research component that will allow it to properly justify IGPE and other institutional investments. FSC research should have excellent overlap with the proposed strategic investments and should act as a bridge between science and programs.

A synthetic chemist works to link two molecules, each of which binds to one protein binding site.

Scanned probe imaging is spread over many labs and is used both for biological applications as well as more traditional physics and materials sciences problems. Generally, applications in biomolecules require the highest resolution and, often, BSL-2 approved operation. CMS has a strong record of scientific accomplishment in this area but no facility that satisfies the BSL-2 requirements. CMS should consolidate much of its scanned probe capability into a biomolecular imaging center that is co-located with a nuclear magnetic resonance center and the nanoSIMS Center.

The BPAC lacks a unified physical identity, in part because of its fragmented real estate that is inevitable because of the range of applications outside CMS. The costs and lost opportunities associated with unifying this capability outweigh the probable benefits.

A strategic decision will be made soon regarding the level of biosecurity work to be supported at Livermore. From a CMS perspective, all crucial needs can be met with surrogates, and it seems likely that the advantages of dealing with real agents as opposed to surrogates will diminish over time.

Interface to engineering: Systems integration is a major challenge in sensing systems. Currently, tooling capabilities for integration in Livermore Engineering are ad hoc. Considerable investments have been made at Sandia National Laboratories and at user fabrication facilities that exist both locally and nationally. Stronger partnerships with regional centers should be developed to provide access to standard electronic-materials processing and tools. Ideally, Engineering will provide a small set of core capabilities on site, and these capabilities should be expanded. Systems testing is crucial for developing prototypes. A testing capability should include an aerosol test facility and the ability to expose sensor systems to "realistic" environments.

Computational biology: A recurring theme in choosing problems to run on Livermore's Blue Gene/L supercomputer is leveraging the phenomenal potential of the new machine. How to efficiently and simultaneously use the 64,000 processors is a huge challenge that CMS is tackling only for inorganic materials. CMS has a strong focus to build fully parallel codes in the area of dislocation dynamics. A similar effort should be in the area of science at the intersection of chemistry, biology, and materials science. Although considerable work has been done to develop efficient, fully parallel codes for materials science problems, little has been done in molecular flow and separation on Blue Gene/L. Developing these codes should be a priority, with Engineering taking the lead. In particular, we should generate biochemically predictive models. The Computation Directorate is building needed algorithms, but they do not include CMS vision or applications. Such modeling is central to efforts to design ligands, to understand backgrounds quantitatively, and to leverage investments in Blue Gene/L.

This researcher is modifying proteins by introducing engineered amino acids.

BioSecurity and Nanosciences Laboratory: Life at the Nanoscale

The BioSecurity and Nanosciences Laboratory (BSNL) was created in 1999 with a simple vision in mind: to provide a dynamic and vibrant environment that could nurture and support the success of good ideas for exploratory science at the boundaries of chemistry, materials science, and biology in support of the Lab's missions in nonproliferation, counterterrorism, life sciences, and energy. At the time, the BSNL was a novel undertaking that involved a significant amount of risk.

The CMS Directorate, in partnership with NAI, BBRP, E&E, and the office of the Lab's Deputy Director for Science and Technology undertook a coordinated and well-planned series of discretionary investments in a new area of multidisciplinary science where the Lab´s emerging missions were not yet fully defined but where there was clear potential for tremendous growth and impact in the future. CMS and the Laboratory have invested significant LDRD and other discretionary resources in launching new exploratory activities and in creating what today has become a world-class capability in bioanalytical science, including state-of-the- art mass spectrometry, nanoSIMS, bioimaging, and nuclear magnetic resonance capabilities.

Those decisions and investments now appear as a clear example of outstanding strategic planning as the BSNL is proving itself an important national asset in the fight against bioterrorism by discovering new methods to detect, identify, image, and understand pathogens such as viruses, bacteria, and their spores. BSNL research findings are also helping improve human health by providing a better understanding of pathogens and molecular machines such as DNA and proteins. In addition, BSNL researchers are already contributing to the Department of Energy's Genomics:GTL Program, the follow-on effort to the Human Genome Project, and are poised to have a major impact in that program as well as in other nascent programs within the Office of Basic Energy Sciences at DOE.

BSNL's 62 researchers are drawn principally from CMS, with significant contributions from the BBRP, Engineering, E&E, NAI, and PAT directorates. More than half the researchers are less than 35 years old. From the start, BSNL managers adopted a strategy of investing in young talent. The center has attracted four Lawrence fellows, who are some of the most sought after young Ph.D.s in the world, and a tremendously talented team of postdoctoral researchers. In addition, the vibrant scientific environment of the BSNL attracts faculty members from around the country to collaborate with its researchers.

Multidisciplinary research teams in the BSNL work at the intersection of biology, chemistry, physics, and materials science. BSNL researchers work to exploit the natural synergy between nanotechnology and new frontiers in biological research in several areas. One of these areas involves understanding the process by which living organisms use biomolecular controls over crystallization to produce materials solutions to their functional requirements. Another area concerns the understanding of protein complexes—the machines that carry out cellular function. The principles that take us from structure to function of protein complexes are largely unknown, as are those that enable protein complexes to turn chemical gradients into work. Yet another area of interest is biomimetics, the science that relies on biologically driven assembly for creating new, functional materials. Examples include the synthesis of nanostructured materials such as artificial membranes with nanometer-sized pores; microfluidic channels that guide the flow of single molecules for analysis; chemical patterning of surfaces with nanometer

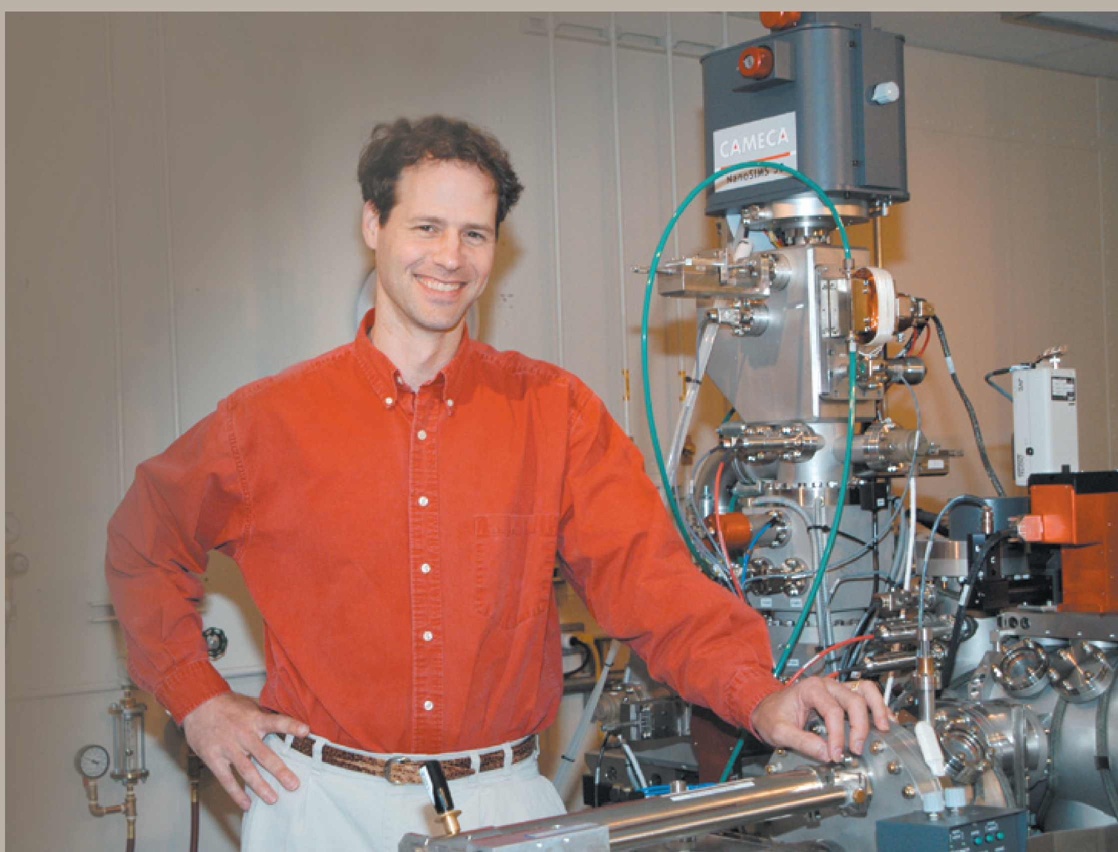
(Continued on next page.)

BioSecurity and Nanosciences Laboratory: Life at the Nanoscale (continued)

precision; and chemical compounds that recognize or bind to specific targets such as toxin molecules.

BSNL researchers have placed special emphasis on work on the single molecule scale, to understand the organization of molecular complexes such as spores, viruses, DNA, or proteins. At the nanoscale, experimental results are viewed with the most powerful imaging techniques, such as atomic force microscopy, scanning probe microscopy, confocal optical microscopy, and nano secondary-ion mass spectrometry. These devices can image and manipulate single molecules, allowing researchers to study a molecule's structure and function. Synthesis methods include traditional small-molecule techniques to produce synthetic high-affinity ligands, which bind to pathogens and render them harmless, and using cells as chemical factories.

By any standard, BSNL is meeting its goals to become a formidable resource for advancing national biosecurity, improving human health, and understanding the molecular machinery of life. Increasing funding from sponsors, a growing number of publications in major peer-reviewed journals, and deepening scientific understanding of pathogens and biomolecules all speak to its success.



The BSNL has a new secondary-ion mass spectrometer (nanoSIMS) that is allowing researchers to interrogate subcellular structures using isotopically labeled compounds. The nanoSIMS has already enabled CMS scientists to initiate research into previously inaccessible areas of nuclear and bionuclear science.

Applied Nuclear Science for Human Health and National Security

This research theme focuses on scientific leadership in radiation detection, radiochemistry, and isotopic characterization. We provide nuclear diagnostics for stockpile stewardship and the National Ignition Facility; identify nuclear signatures to detect, identify, quantify, and attribute nuclear materials; and shape new Laboratory programs through innovation and discovery in nuclear science.

Vision

To advance nuclear science techniques for scientific discovery and technology development that support stewardship of nuclear materials, national security, and improvement of the human condition.

We want CMS to be the "go-to" organization for radiochemical, isotopic, and spectroscopic nuclear analysis at the Laboratory, and to be internationally recognized for paradigm-changing discoveries using nuclear-science tools.

Strategies for Change

Achieving this goal requires that CMS build on its strengths in mass spectrometry, neutron and gamma-ray detection and imaging, spectroscopic analysis, radiation transport simulations, advanced signal processing, and certified counting techniques. It also requires that CMS recruit outstanding scientists from the decreasing pool of nuclear scientists, which poses an additional challenge in nuclear science. Our strategy is to attract and retain the best talent by strengthening our reputation as an international center of excellence.

CMS has identified three strategic objectives for applied nuclear science:

- Supporting existing Laboratory programs in Defense and Nuclear Technologies (DNT); Nonproliferation, Arms Control, and International Security (NAI); Energy and Environment (E&E); and Environmental Protection (EPD).
- Enhancing leadership in nuclear science and technology by developing new initiatives that use radiation detection, isotopic analysis, and radiochemical science in paradigm-changing scientific discovery.
- Playing a leadership role in emerging national security missions, including homeland security and diagnostics at the National Ignition Facility (NIF).

Applied Nuclear Science Capabilities

The applied nuclear science theme area uses radiochemistry, isotope analysis, radiation detection, and simulations to solve problems in the national interest. Among its traditional functions are to support the safety and reliability of the nuclear stockpile and help counter terrorism and deter proliferation of nuclear weapons. To accomplish these tasks, ANS works primarily with the DNT and NAI directorates. To a lesser extent, the division has supported E&E and EPD as they tackle environmental problems affecting nuclear waste cleanup and drinking water safety. ANS also works with BBRP in applying radiation science to improving human health. The Glenn T. Seaborg Institute, described on p. 44, plays a key role in applied nuclear science research.

A CMS geochemist collects groundwater samples in central Nevada for stable isotope analysis.

Glenn T. Seaborg Institute: Nuclear and Bionuclear Science in the National Interest

The Glenn T. Seaborg Institute was established in 1991 to foster research in fundamental and applied nuclear science and technology. Our goal is to enhance the impact of nuclear and bionuclear science on important national problems such as homeland security, health, and the environment.

The Institute is also committed to the training and development of future generations of nuclear scientists needed to address the national problems. Our target population for this commitment is students and teachers from high schools, junior colleges, and undergraduate and graduate programs at colleges and universities. Our work to develop a future pool of talent is of current and growing importance not only to ANS but also to efforts throughout CMS.

The nuclear and bionuclear science efforts at the Seaborg Institute focus on the following:

• Contributing to the safety and reliability of the nation's nuclear weapons stockpile by supporting the Department of Energy's Stockpile Stewardship Program.
• Helping to counter terrorism and deter the proliferation of nuclear materials.
• Applying radiation science research on ways to improve human health.
• Using isotope tracking and actinide chemistry to tackle environmental problems affecting drinking water safety and nuclear waste cleanup.

Other work of the Institute includes ongoing studies of nature's newest elements and efforts to improve the accuracy and effectiveness of molecular targeted radioisotope therapy for advanced cancer. Overall, we are striving to enhance public understanding and student involvement in nuclear science.

Students from the 2002 Nuclear Science Internship Program, which provides the next generation of nuclear scientists, with mentors and career support.

Strategic Objective

We will strengthen our capabilities in support of several Livermore programs as they fulfill their DOE missions. For DNT, CMS scientists provide expertise in stockpile radiochemistry to ensure the safety and reliability of the nuclear stockpile. For NAI, CMS experts support programs in treaty verification; nuclear material safeguards and inventory control; materials protection, control, and accounting; IAEA technical support; basic research for nonproliferation; and highly enriched uranium transparency. CMS researchers tackle environmental problems affecting drinking water safety and nuclear waste cleanup with E&E and operate a full radioanalytical facility for clients such as EPD, supporting both waste characterization and environmental monitoring.

Program Challenges

Stockpile radiochemistry: CMS is reinvigorating its long-term relationship with DNT programs through the auspices of the Stockpile Radiochemistry Group, which is integral to the success of DNT. Achieving major milestones in stockpile stewardship depends on providing improved radiochemical diagnostic interpretations of historical nuclear test data. The fidelity with which explosion codes can predict the performance of an untested device is estimated by the ability of those codes to model the data taken during nuclear tests. Uncertainties associated with device yields reported by radiochemistry are the controlling factor in constraining the calculations. Fully one-quarter of the technical measures of success spelled out in Appendix F of the LLNL contract rely on improved radiochemistry. We are continuing to refine our understanding of DNT's program needs for more stringent constraints on the radiochemical data, as the program simultaneously develops better codes with higher fidelity.

Radioisotope detection for national security and arms control: The Material Protection and Accountability (MPC&A) Program and highly enriched uranium (HEU) transparency program require a highly reliable field radiation detection capability in Russia. CMS expertise ranges from isotopic analysis using high-resolution gamma-ray spectroscopic systems to isotopic verification with low-resolution "enrichment meter" systems. For future support of NAI, CMS needs high-resolution, high-efficiency, room-temperature spectroscopic detectors in conjunction with intelligent isotopic analysis engines to provide automated, remote-sensing, uncertainty-reduction capabilities.

Environmental radiochemistry: For E&E, CMS has considerable experience in vulnerability assessments involving a broad range of contaminants. For Laboratory site operations clients, CMS is the repository of applied nuclear knowledge and analytical capability, primarily through the CMS Chemistry Environmental Services (CES) Group. CES not only analyzes the majority of wastes created at LLNL but is also responsible for determining if materials are to be managed as radioactive or nonradioactive. The environmental radiochemistry group supports LLNL through environmental site monitoring and is regarded as a national resource in analyzing the fate and transport of radioactive materials.

CMS sustains the core capabilities of radiochemical debris analysis and device diagnostics in support of DOE stockpile stewardship and required test readiness.

S&T Challenges

Stockpile radiochemistry: The stockpile radiochemistry effort requires improved cross-section sets for the reactions of thermonuclear neutrons with detector materials. It also needs improved measurements of the yields of the end-member products produced in the fissions of each of the nuclear fuels. The magnitude of this task is daunting. For example, the cross-section set for the reactions of neutrons with lutetium (a common thermonuclear detector) to produce both multiple-order (n,2n) and (n,_) products involves 175 crosssections. There is experimental data for only five of the reactions; the rest of the cross-section set is completely calculational. The lutetium set is considered to be one of the more reliable ones available to the group; the cross-section data of 24 other elements are in much worse shape. Improved thermonuclear yield diagnostics require measurements of the reactions of neutrons with short-lived target nuclei and an improved modeling effort.

This DNT-centered effort is synergistic with the needs of both the Defense Treat Reduction Agency (DTRA) Domestic Nuclear Explosion Project and N-Division plans for the Rare Isotope Accelerator (RIA). For the DTRA project, accurate cross sections are necessary to reconstruct the preexplosion isotopic composition of the fission fuel of a potential terrorist device from the residual actinide materials in the debris of the explosion. Without appropriate cross sections, it will be impossible to extract the subtle differences in the concentrations of preexplosion signature nuclides with enough fidelity to assign responsibility. N Division is planning to construct a neutron source at RIA to measure cross sections for reactions with short-lived radioactive species. These experiments rely heavily on radiochemistry to harvest the primary RIA product and fabricate it into targets.

The radiochemical diagnostics of nuclear explosions extend directly to the study of the performance of fusion capsules in NIF. Radiochemistry provides the means to extract the amount of fuel/shell mixing caused by spallation and the microscopic imperfections due to machining and fabrication. Charged particle interactions with loaded radiochemical detectors provide information on the scale of mix, just as they did during the days of nuclear testing. When the NIF experimental program begins to achieve ignition, it is expected that any failure may result from an incomplete knowledge of mix phenomena.

Environmental radiochemistry: As the LLNL resource for characterizing radioactive wastes, CES needs to develop three technologies. The first is a rapid, high-throughput analytical method for measuring alpha emitters at picocurie detection limits in a variety of matrices. The second is a nondestructive assay to identify and quantify the amount of radioactive contamination in large items. Finally, a fieldable, real-time detection technology is needed for detecting radionuclides, regulated metals, and organic compounds.

Technicians collect water samples at the Nevada Test Site. Mass spectrometry and radiochemistry will then help them determine the fate and transport of anthropogenic radionuclides.

Strategic Objective

Our goal is to enhance CMS's role as the "go-to" organization at the Laboratory for radiation detection, isotope analysis, and radiochemical science and technology. CMS fosters scientific excellence in key relevant disciplines, which strengthen our ability to attract the best and brightest talent for new and existing national security sponsors.

CMS seeks to be a leader in the science of nuclear signatures. There is increasing recognition of the importance of tracing natural and man-made isotopic, elemental, molecular, or cellular fingerprints to provide insight to nuclear, chemical, or biomedical processes important to national security, the environment, and health. Understanding the source of these fingerprints, their chemical properties, persistence, and evolution, and developing tools for detecting them are essential to fully exploiting their diagnostic potential.

Program Challenges

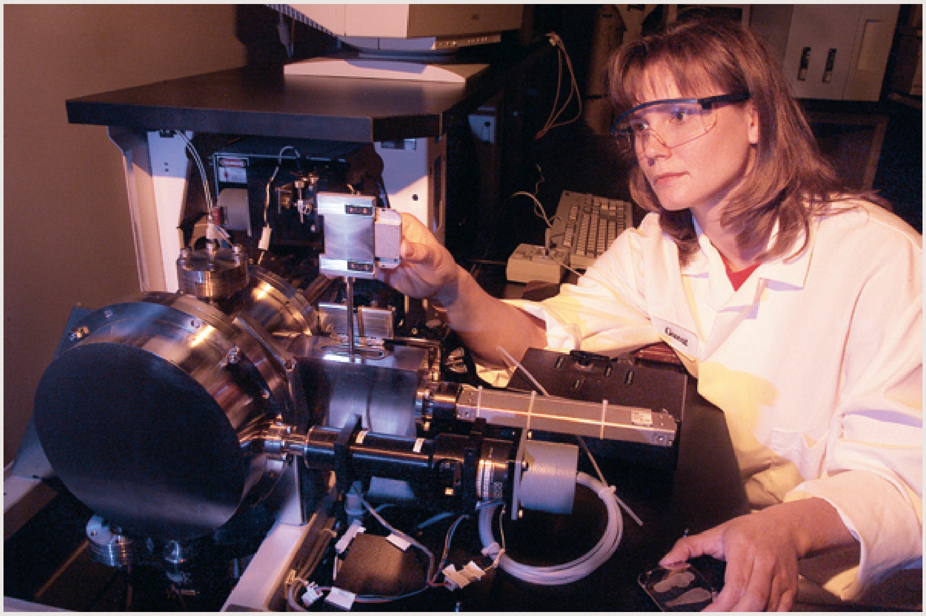
A major challenge is to develop programmatic sponsorship for peer-reviewed nuclear science activities. CMS is developing scientific sponsors such as the National Institutes of Health, OBER, and OBES, with an overall strategy of partnering with recognized (and funded) leaders and bringing unique skills and equipment to LLNL.

S&T Challenges

Over the next year, a major CMS goal is to develop a strong applied nuclear science identity that synthesizes CMS strengths and capabilities to foster paradigm-changing research and discovery. To identify new scientific questions, we will network with nationally recognized scientists and build collaborations with universities and leading national centers. As research thrusts develop, we anticipate the development of a new experimental nuclear science facility that serves as a unifying force for applied nuclear science researchers. Below are some capabilities that we will bring to bear on new scientific questions.

Bionuclear science: CMS is developing a state-of-the-art capability to perform bioanalytical chemistry in support of Livermore's growing missions in biological counterterrorism and human health. This effort, which involves the colocation of existing capabilities and substantial technology investments, will create a robust scientific environment with strong links to Livermore mission areas and will serve as an attractor for new talent into CMS.

Gamma-ray imaging: Gamma-ray imaging is viewed as a key enabling technology in national security and basic nuclear science, as researchers have recognized the role of spatial localization in improving the signal sensitivity of the system. Advances in solid-state detector technology, combined with fast signal processing, make it possible to build collimator-less imaging devices that promise 100 times more efficiency over systems requiring collimators. If these new imagers live up to their promised efficiency and can be built in sufficiently rugged systems, they promise to revolutionize radiation imaging for medicine and national security.



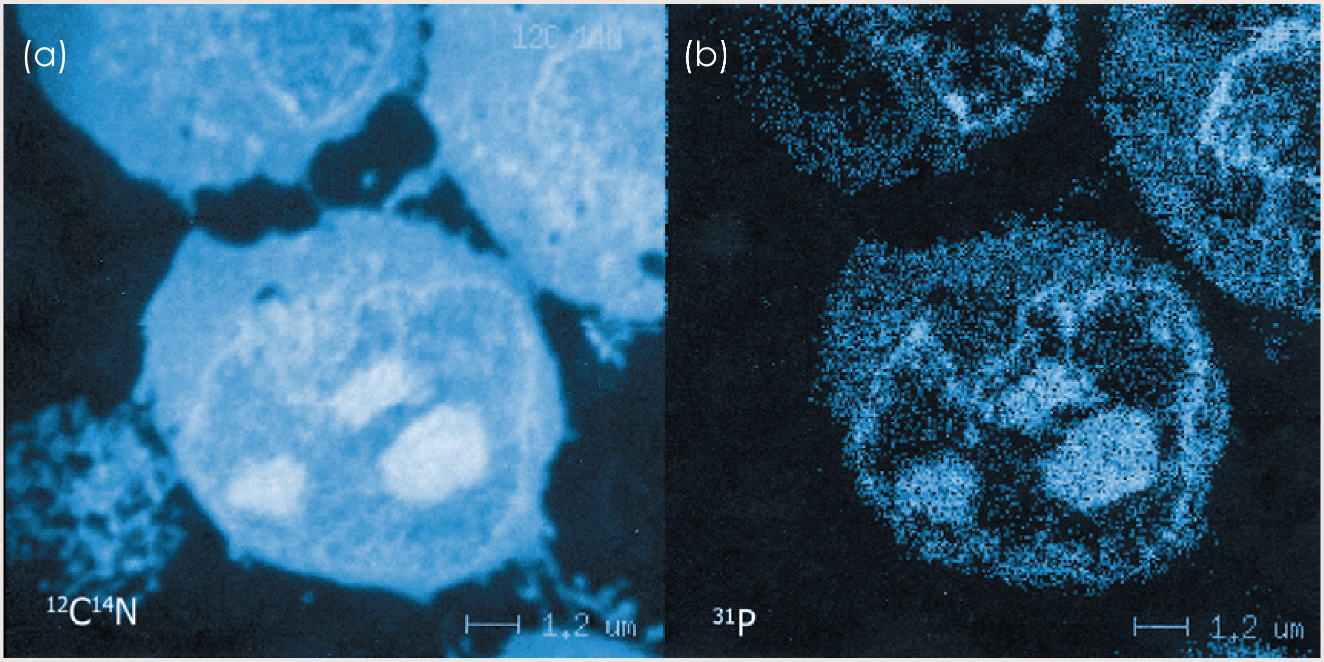
Laser-based spectrometers assist in identifying large biomolecules in their natural environment.

New-generation radiation detectors: High-resolution radiation detection technology currently suffers at room temperature, and flexibility and ruggedness issues remain as well. For CMS to be ahead of the competition, assessing the potential for developing new materials for radiation detection is a must. With recent advancements in nanotechnology, it is likely that higher scintillation efficiency and better charge collection will dramatically improve radiation detection capability.

One completely new form of radiation detection relies on the biological response of cells to radiation as a way to rapidly detect radiation dose after exposure has occurred. Cellular response consists of the up-and-down regulation of messenger RNA (mRNA) and increased or decreased presence of proteins and small molecules. These changes themselves could be engineered into a biologically based detector. Because of the importance of mass spectrometry in identifying protein and small molecule changes, CMS's role in this research is pivotal.

Synergistic experiments and simulations: The development of new detectors and detection concepts relies heavily on Monte Carlo radiation simulations as a design tool. Researchers in CMS have substantial experience and an outstanding track record for integrating these simulations into the design process. These efforts will be strengthened and expanded to streamline the detection system design process.

Cutting-edge imaging with mass spectrometry: CMS recently acquired a secondary-ion mass spectrometer (nanoSIMS) that defines the technological cutting edge for spatially resolved isotope and trace-element measurements. It has already enabled CMS scientists to initiate research into heretofore inaccessible areas of nuclear and bionuclear science. Projects revealing the history of the first 5 million years of the solar system, developing new isotopic signatures indicative of the processes and growth sites of biological weapon agents, and using variations in O-isotopes to determine the geographical locations of nuclear fuel manufacturing and reprocessing sites would not be possible without nanoSIMS. This work augurs well for the future of nuclear science at LLNL and our ability to attract the best and brightest new talent.



Images of 8-micrometer Raji cells taken using the nanoSIMS with a spatial resolution of approximately 50 nanometers. Distributions of (a) nitrogen and (b) phosphorus are apparent as ovoid-shaped bright regions in the center of the cells.

Strategic Objective

Our goal is for CMS's roles in DNT, NAI, NIF, and the Department of Homeland Security (DHS) to serve as a core around which we will maintain scientific leadership, nurture new initiatives, and expand our customer base.

Program Challenges

New national security customers: DHS has programmatic needs that align with our capabilities in applied nuclear science, although it remains unclear how DHS will work with LLNL in many research and development areas. However, DHS recognizes LLNL as a key laboratory supporting its R&D and operational missions and has already established programs at LLNL in radiological and nuclear countermeasures. These programs include the Nuclear Assessment Program, the Port Authority of New York and New Jersey field test operations, and several detector development projects. Although DHS tends to focus on relatively short-term programs, with an emphasis on transitioning technology to field use, long-term research opportunities are likely to spin off, particularly if they can be coordinated with higher-risk research activities funded through other sponsors.

Livermore is recognized as a leader in nuclear attribution. The new focus on countering terrorism has highlighted the importance of nuclear attribution, and CMS is poised for enormous growth in the funding for this research.

Similarly, CMS scientists have emerged as leaders in the development of Livermore's consequence management proposals to DHS. In the area of medical assessment and treatment, CMS has collaborated with BBRP to create a proposal for plume and dose forecasting. CMS has led an effort to link previously separate efforts in weapons effects, plume modeling, environmental transport, and risk assessment. This initiative, unique among the DOE laboratories, fits well with the new CMS thrust in chemical biology.

The combined resources and expertise of CES and the Forensic Science Center (FSC) (See sidebar on pp. 35–36) form a strong team for consequence management. CES, which specializes in moderate complexity analyses at a high-throughput level, already has a mature and robust sample management capability. The FSC specializes in high-risk, high-complexity analyses, typically of one-of-a-kind samples. A partnership between these two organizations creates substantial opportunities for Livermore to extend its leadership in forensics into areas that require complex analyses but at a much higher volume than the FSC can currently handle. Perhaps the most notable success in this partnership was Livermore's recent certification by the Organization for the Prohibition of Chemical Weapons, only the second such institution in the country to receive this certification.

NIF nuclear diagnostics: The NIF laser fusion machine is slated to operate at LLNL for the next 30 years. The construction and calibration of suitable nuclear diagnostics for NIF, especially for the ignition campaign starting in 2009, is a potential growth area, and substantial increases in programmatic funding should be expected within the next few years. With proper planning, CMS will take leadership roles in this effort. Two areas of opportunity can be identified:

Radiochemical diagnostics: CMS is the unique and sole provider of radiochemical diagnostics to NIF. Radiochemical diagnostics involve collecting target debris via collector foils or gas sampling systems and subsequently counting the radioactive species, as opposed to prompt diagnostics that give immediate results in real time. Radiochemical

Chemistry Environmental Services has the only certified laboratory that can assay radioactive materials throughout DOE.

diagnostics also include the collection of activated solid materials for total yield analyses. These diagnostics are important because some of the fusion products may be accessible only by radiochemical means. Areas of research will include capsule development for the seeding of tracer elements into NIF ignition targets; new and better schemes for collecting the target debris; and new methods for determining total yield from activated solid samples.

Prompt diagnostics: Existing laser fusion facilities rely heavily on prompt diagnostics, and NIF likely will as well. Prompt diagnostics research will include the development of solid-state detector and scintillator time-of-flight systems for neutron spectroscopy; segmented detector arrays for neutron imaging and/or backlit proton radiography; ultrafast sensors for burn history measurements; and neutron detector calibration methods, especially for the important downscattered neutron region ($E < 14$ MeV). Monte Carlo radiation transport simulations will aid with instrument design, calibration, and data analysis. These research areas overlap well with existing expertise and R&D in NAI, DNT, and the radiation detection sections of CMS.

S&T Challenges

New national security customers: DHS research needs align with many of our own capabilities. They include developing improved radiation detection equipment and radiation identification methods; systems integration and performance assessment; high sensitivity methods, particularly for the detection of special nuclear materials; radiation imaging; field applications of radiation detectors; active interrogation methods for the detection of special nuclear materials; high accuracy quantitation of radionuclides in irregular/arbitrary-shaped containers by nondestructive means; radiation transport and detection simulations; integration of radiation detection capabilities with other intelligence and law enforcement assets; and extremely high-confidence radiochemical analyses of unique samples for law enforcement or other reasons.

NIF diagnostics: CMS should pursue many fundamental science and technology issues associated with NIF, including target doping and chemical fractionation studies for radiochemistry experiments and for comparison to underground test data, new detector materials for neutron sensing and imaging, techniques for neutron detector calibrations at unusual energies, and cross-section measurements of important activation reactions and/or reactions of fast neutrons with candidate tracer nuclei. We can also investigate ways to use NIF itself for cross-section measurements. Any project associated with NIF, the highest profile project at the Lab, can serve to attract new talent to the directorate and to help in recruitment.

Workforce Requirements

Livermore has lost significant expertise and experience in applied nuclear science in the last two decades. Changes in funding priorities in basic science and a decline in the prominence of basic nuclear science have resulted in a drastic decrease in the number of nuclear scientists receiving degrees from U.S. universities. In just the last decade, the number of university nuclear engineering programs and undergraduate enrollment in these programs has decreased by 50 percent. NNSA laboratories face stiff competition for recent graduates from the medical and nuclear industries and from state governments and non-NNSA federal institutions. These trends threaten the long-term viability of traditional NNSA missions and limit the development of new nuclear national security programs.

Attracting students to nuclear science: To address this shortfall, we are developing a nuclear science education and recruitment program that reaches into a diverse undergraduate population, supports graduate study in nuclear science, and recruits promising Ph.D. graduates and postdoctoral fellows. Undergraduates are recruited from a wide range of colleges and universities. For graduate studies, we are maintaining a close relationship with targeted graduate programs that have a track record of producing excellent graduates in applied nuclear science. These education and recruitment efforts are accomplished through programs managed by Livermore's Glenn T. Seaborg Institute (see sidebar p. 44.) and participating ANS scientists.

Training next-generation event nuclear chemists: To meet the challenge of supporting DNT despite waning numbers of personnel with actual underground test experience, we have begun training two new event nuclear chemists. Traditionally, this job has been to ensure that the radiochemical loadings in the explosive device accomplished the goals of the designer, that the proper measurements are made by the radiochemistry division, and that the final data are synthesized into a device performance report. The job called for enormous chemical, physics, and engineering expertise acquired through experience and informal mentoring, which has not been possible to sustain since the end of testing. However, through carefully designed exercises and training, young scientists relatively new to the program are now making major contributions to the DNT effort, despite never having managed an underground nuclear test.

Widening the science net: CMS strives to broaden the expertise it applies to DNT problems through strategic partnerships with other program elements and by educating new staff on the basic science needed for stockpile stewardship and nuclear science programs. The critical skills essential for these two missions are also central to nuclear science applications in energy, environment, and health. Skills developed during the nuclear testing era are central to our efforts to counter the smuggling of nuclear materials and to attribute responsibility for a domestic nuclear explosion. Extension of traditional radiochemical analysis to NIF capsules will allow us to mine small samples of debris from a spent NIF capsule and determine important details about the scale of mix at fuel–shell interfaces that cannot be determined any other way.

Expanding opportunities in environmental radiochemistry: CMS's nuclear science expertise can provide personnel for leadership roles in EPD. More formal interactions between CES and EPD leadership will benefit both organizations. For example, CES and environmental radiochemistry currently offer subject-matter expertise in the release of radioactive materials and requirements for sampling and analysis of many types of waste. In addition, top CES and environmental radiochemistry managers are becoming recognized as national experts in the areas of waste sampling and analysis and analytical facility management.

Supporting the Department of Homeland Security: CMS scientists played a strong role in developing a vision for a DHS system of data management and technical reachback for its deployed nuclear detectors. This system, configured as part of an expanded nuclear assessments program, could grow rapidly if it is not limited by the availability of radiation detection experts. Reassignments and new hires must be pursued. CMS should also continue to seek to place leaders with program development and operational skills in this program. To build strong, lasting ties with DHS, CMS expects to continue assigning key staff to the DHS organization in Washington, D.C. In early 2004, a former division leader and a program manager were working as portfolio manager and program manager in the DHS Science and Technology Program.

To better address issues related to nuclear attribution, CMS must assemble a core group of scientists from radiochemistry, mass spectrometry, geochemistry, and nuclear technologies. For success and growth in our nuclear capability, CMS is reaching out to disciplines in other directorates to build teams that will allow growth in both scientific contribution and programmatic value. Additional staff members are also required in neutron spectroscopy, radiation imaging, detector materials, detector electronics and data acquisition, rapid prototyping, radiation simulation for reverse engineering of signals, signal processing, systems integration, and field experiments. Key partnerships will help these areas grow.

Infrastructure Requirements

Dissolver wing: Building 151's dissolver wing is a core capability for Livermore's stockpile stewardship activities. Should the U.S. resume nuclear testing, Livermore must be prepared to serve as the primary radiochemical diagnostics laboratory within the nuclear weapons complex. The dissolver wing houses a custom glovebox chain in a vault-type-room laboratory and a system for pulverizing and dissolving nuclear melt glass cores from underground tests. CMS periodically exercises this capability for the weapons program as a readiness deliverable. CMS also uses the dissolver wing to support other programs that require transient use of vault-type laboratory space.

Training young scientists how to evaluate core samples for stockpile stewardship.

Because the facility is often idle, CMS is adapting the protocols and procedures for the dissolver wing to augment other programs. As an example, the system is being adapted to accommodate samples that may be taken from a terrorist event. Such samples could be substantially different from the samples acquired for the diagnosis of underground nuclear tests, which will require modifications in handling and chemical processing procedures.

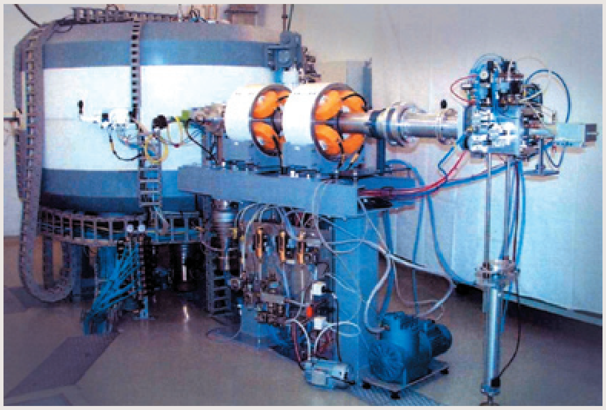
A unifying nuclear science facility: Acquisition of a small medical cyclotron to be installed in the dissolver wing will advance efforts in radiochemistry and detector development and help to link these two traditional strengths. Investment of $1–2 million in a small accelerator capable of generating beams of protons and deuterons would make our division central to several efforts at the Laboratory. With a source of monoenergetic protons and neutrons, we can calibrate detectors for NIF and NAI applications. With a source of radionuclides, we can provide materials for synthesizing medical isotopes, novel tracer applications, and radiochemistry procedure development in stockpile stewardship and environmental sciences (including CES). Stockpile radiochemistry would also use the machine for mission-critical fission-product measurements. This new capability will also make Livermore an attractive facility for the training of a new generation of radiochemists.

Environmental radiochemistry: The CES laboratory, which holds the largest concentration of chemical and radiochemical analytical instrumentation at LLNL, has had difficulty investing in laboratory space and new instrumentation. The CES Group must develop a workable capital investment strategy that takes into account current client needs and plans for future growth and maintenance of needed analytical capabilities. For the foreseeable future, CES will be the repository of general analytical chemistry in CMS and should be supported at a level sufficient to maintain vital capabilities.

Additional laboratory requirements: For CMS to remain a leader in radiation detection, radiochemistry, and isotopic characterization as the world continues to change, we must make investments in several key areas. We need development laboratories for novel materials, detector assembly and testing, and rapid prototyping capabilities. An important requirement is the ability to challenge detectors with quantities of radionuclides, especially special nuclear materials, that provide statistically significant samples.

We also need high-quality radiochemistry labs and radiation counting labs with top-line capabilities in gamma spectroscopy, facilities capable of handling or producing sources for active interrogation, test assemblies for special nuclear materials and surrogates for detector challenges, outdoor experimental test capabilities for assessing "drive-by" detector performance, and simulated or mocked-up port cargo handling equipment.

The dissolver wing in Building 151 houses a facility for processing highly radioactive samples.



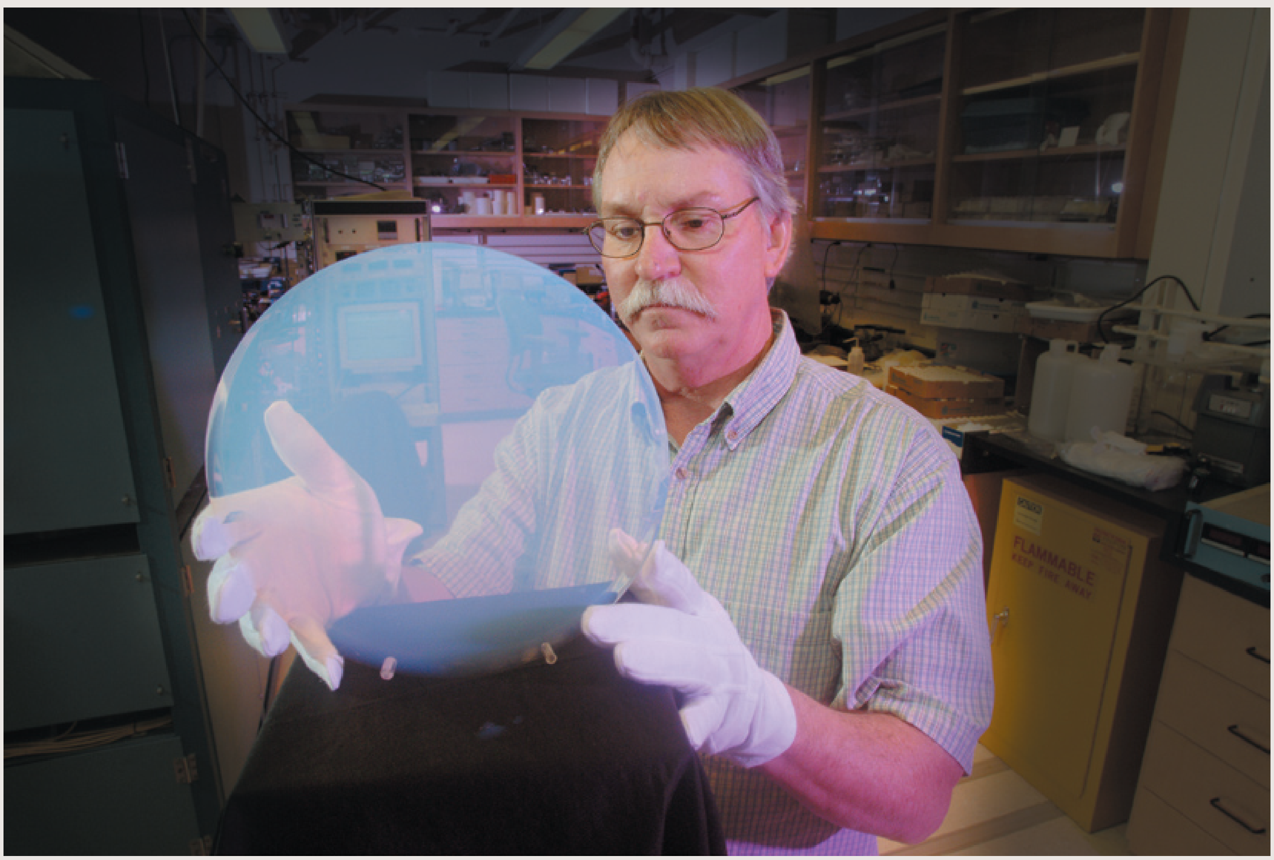
The small medical cyclotron to be installed in the dissolver wing in Building 151 will be similar to this one.

Agility and Flexibility Are Keys to Meeting Challenges of Changing Environment

Long-range planners must be prepared to alter their plans to meet ever-changing situations and conditions. For this reason, a key guideline for preparing the CMS Strategic Plan is that it enable the directorate to be agile and flexible so it can both recognize and respond to change.

An important ingredient of being agile and flexible is maintaining the intellectual vitality of our staff. We intend to do this by expanding our collaborations with others in the scientific community and by attracting the best possible young scientists and engineers through our postdoctoral, academic alliance, and other programs. These efforts will enliven our directorate with new ideas, and keep us poised to respond to changing conditions. (See related sidebars)

We understand the importance of agility and flexibility when we see how frequently change takes place in leadership and in the scientific and technical environment in which the Laboratory and the CMS Directorate operate. For example, just since the start of 2002, a new director has taken office, and several new associate directors have been appointed. New people have assumed key positions at the Department of Energy (DOE), the National Nuclear Security Administration (NNSA), and the University of California (UC). And the relationship of UC to its national laboratories has been scrutinized as never before.



We have successfully synthesized ultra-low-density aerogel at 1 mg/cc, setting a new world record.

In addition, the U.S. Department of Homeland Security was established, and the Laboratory created a homeland security organization of its own. Physical- and cyber-security requirements have become more stringent at Livermore. The internationalization of science and technology poses increasing challenges to the Laboratory in terms of staffing and external partnering, particularly because of security concerns.

Conditions have changed on many other fronts as well. The country has been fighting a war. The threat of nuclear, chemical, and biological terrorism redefines and magnifies the importance of many disciplines, including forensics. Technical demands on the weapons program are increasing as the need grows for nuclear weapon refurbishments and as the impact becomes clearer of weapon requirements resulting from the Nuclear Posture Review (the annual review of the U.S. arsenal). Congressional discussions are focusing on a perceived need to develop new low-yield nuclear weapons.

Other changes will result from the 2004 presidential and congressional elections and perhaps from the need for UC to compete to retain management responsibility for its laboratories.

At the Laboratory, the National Ignition Facility is making the transition from a construction project to an experimental tool for stockpile stewardship and basic science. The importance of large-scale simulation and computing will continue its rapid growth with the delivery of the Advanced Simulation and Computing Program's ASC Purple, a machine capable of 100 trillion operations per second that will be used primarily for classified work. Similarly, unclassified computational capabilities are growing at Livermore, providing unprecedented high-performance computing access to researchers in nonweapon areas. The effects of the enormous growth in computations are already being felt in areas such as materials science, environmental science, and biology.

In addition, in the scientific community at large, scientific and technical discoveries and inventions appear daily, many in areas of direct interest to LLNL. Examples include actinide science, biological and chemical weapons technology, and rapidly advancing information technology capabilities.

Finally, we must be prepared for another aspect of change. The Laboratory and its scientists are important agents of change as well as responders to change. Our ideas, inventions, and discoveries often affect the way we and others think about the world. Although we can't plan scientific breakthroughs or discoveries, we can manage the environment that cultivates them and manage how we respond to them. Our responsibility is to create an environment where discovery and invention are possible and then to quickly recognize and nurture their potential, no matter where they originate.

This sampling of changing conditions and situations forms the backdrop for CMS strategic planning. Change will always be with us—some anticipated, some unexpected. That is why the directorate places so much importance on being agile and flexible. And it is why our planning will be reviewed regularly, and priorities and focus altered as needed.

I wanted each member of the CMS Team to have a copy of the plan so it could be read and referred to over time. It will help each of you better understand the strategic directions of the Laboratory and CMS so that you can contribute fully to both, today and in the future.

Thank you for reading this plan,

Tomás Díaz de la Rubia

Academic Alliances Sustain Flow of New Ideas

Sustaining our scientists' intellectual energy and a flow of new, exciting ideas from the scientific community at large are key objectives to ensure that the CMS Directorate fulfills its vision and accomplishes its mission. A strategy to realize these objectives is to establish focused, long-term academic alliances and university partnerships. Moreover, the establishment of a vigorous university outreach program ensures that the CMS Directorate remains positioned to attract and retain a workforce for the future. By forging collaborative interactions with talented graduate students early in their careers, we can expose them to the exciting scientific opportunities at the Laboratory in general and within the CMS Directorate in particular.

The CMS Directorate is making strategic investments to support investigators and their graduate students at leading research universities. Involvement by CMS personnel in directorate-supported collaborations helps to ensure that long-term benefits derive from our investments. These efforts will help CMS maintain leading-edge and up-to-date scientific capabilities and recruit a workforce with skills commensurate with the Laboratory's future mission needs and directorate strategic objectives. In addition, the directorate is actively engaged in national-level, NNSA-supported academic alliances programs, including the ASC Strategic Alliances Program and the NNSA Academic Alliances Program. The directorate and the Laboratory University Relations Program also cosponsor summer institutes for undergraduate and graduate students. The institutes allow students to become familiar with Livermore's unique scientific capabilities, forge long-term collaborations with mentors, and develop a lasting image of the Laboratory as an exciting and dynamic science and technology organization that they will aspire to join.

External Sponsors Are a Bridge to Scientific Vitality

An important part of the CMS vision for excellence in science and technology is external sponsorship of many core capabilities. Our external sponsors and work- for-others (WFO) clients range from the Department of Defense (DoD), the National Institutes of Health (NIH), and the Department of Energy Office of Science's Office of Basic Energy Sciences (BES) to industry and organizations in the intelligence, energy, and environmental sciences.

Sponsors other than National Nuclear Security Administration and the Department of Homeland Security are a bridge to the scientific vitality outside the Laboratory. They help to develop our workforce, foster critical external connections, and bring much deserved recognition to our staff. Work for these sponsors leverages off our core technical efforts, allowing us to take greater risks. This scientific exploration of our advanced technologies helps improve core and mission-relevant programs.

There are many examples of how our external sponsors and WFO partners have enriched our scientific and technological world and helped us develop LLNL's science and technology strategies. The DoD's support for exploration and development of high explosives and chemistry under extreme conditions amounts to the largest investment from any external sponsor for Livermore's nanotechnology research. Our growing relationship with NIH helps us stay in the vanguard of one of the fastest growing scientific areas—that represented by the overlap between biology, chemistry, and materials science. NIH funding is a key ingredient in our BioSecurity and Nanosciences Laboratory and may prove to be a pivotal stepping stone to our participation in the DOE's Genomics:GTL activities.

BES has been one of the strongest external sponsors for fundamental science in CMS. The science we do for BES is continually being recognized as our research staff publish in peer-reviewed literature, give invited and contributed presentations, and serve on editorial and advisory bodies. In CMS, most fellows of professional societies have been a BES principal investigator at some point in their careers. Our work for BES is some of the most visible to the outside world. Our external sponsors connect us to industry, universities, and other laboratories that offer new ideas, people, and unique facilities, helping us to enrich our core scientific and technological capabilities. And because the work done for many of these sponsors is highly visible nationally and internationally, it helps attract the best new researchers to the Laboratory. Our externally sponsored scientific and technical activities are vital for our support of the Laboratory's mission and for assuring continued scientific and technological leadership.

Postdocs Help Connect CMS to Broader Scientific World

Postdoctoral researchers remain our strongest conduit to the larger scientific community, and they connect the directorate to the world. The CMS postdoctoral program has more than quadrupled in size over the past five years, and it continues to attract top young talented scientists and engineers to the directorate. When postdoctoral researchers join the Laboratory, they bring new ideas and techniques from universities to solve scientific problems of national importance. CMS's postdoctoral program works to ensure a smooth transition from academia to the national laboratory environment. It also helps to identify long-term career possibilities for outstanding postdocs during their two-year tenure at Livermore. For postdocs whose career ambitions take them from the Laboratory, we ensure that their experience here leads them to recommend the Laboratory to future graduates.

Approximately half the postdocs in CMS are supported financially by Laboratory programs, with the remaining half institutionally supported by the CMS Directorate. These CMS Directorate postdocs are placed strategically into projects that are aligned along research pathways identified by CMS leadership; in this way, additional resources are allocated for postdocs to pursue topics identified with our strategic plan. CMS also has attracted six of the very prestigious Lawrence fellows over the past few years. They have worked primarily in computational materials science and in the BioSecurity and Nanosciences Laboratory. The Lawrence fellows are highly competitive and involve a rigorous selection process. CMS's ability to attract these special postdocs is an indication of the scientific excitement of our programs.

CMS encourages postdocs to pursue research opportunities where they can apply and develop their skills.

A Web version of this strategic plan is available from the CMS Web site. The Plan site also includes information not presented in this document that is relevant to CMS strategic planning. The Plan Web site will be updated periodically to keep CMS employees apprised of important strategic planning issues and proposed future plans for the directorate.

Managed by the University of California
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